REPORT DOCUMENTATION PAGE	Form Approved OMB NO. 0704-0188

Public Reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comment regarding this burden estimates or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188,) Washington, DC 20503.

1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE November 18, 2003	3. REPORT TYPE AND DATES COVERED Final Report (15 Aug., 2002 – 31 Aug., 2003)

4. TITLE AND SUBTITLE **Alloys-by-Design Strategies Using Stochastic Multi-Objective Optimization**	5. FUNDING NUMBERS DAAD19-02-1-0363
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) The University of Texas at Arlington Department of Mechanical and Aerospace Engineering UTA Box 19018 Arlington, Texas 76019	8. PERFORMING ORGANIZATION REPORT NUMBER 26-0401-09-Rep-02
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) U. S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	10. SPONSORING / MONITORING AGENCY REPORT NUMBER 43342.2-MS

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

12 a. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited.	12 b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

The objective was to develop and demonstrate a technique for multi-objective optimization of the chemical composition of steel alloys with the use of an existing experimental database. The technique involves organization and execution of an iterative optimization experiment, which results in a set of Pareto optimum chemical compositions. The algorithms of response surface building known as IOSO was used where the response surfaces are built in accordance with existing experimental information. In a set of experiments the information on alloy properties in Pareto set neighborhood is accumulated, which makes it possible to increase the accuracy of results obtained. After each iteration of this technique, a set of new alloy compositions is formed which are assumed to be Pareto optimal, and for which experiment evaluation of properties should be carried out. For this work, algorithms of artificial neural networks were used that utilized radial-basis functions modified in order to build the response surfaces. The modifications consisted in the selection of ANN parameters at the stage of their training that are based on two criteria: minimal curvature of response surface, and provision of the best predictive properties for given subset of test points. The procedure was demonstrated to work successfully and efficiently.

14. SUBJECT TERMS Multi-objective optimization; Pareto optimum Response surfaces Design of materials; alloy composition optimization			15. NUMBER OF PAGES 57 16. PRICE CODE
17. SECURITY CLASSIFICATION OF REPORT **UNCLASSIFIED**	18. SECURITY CLASSIFICATION ON THIS PAGE **UNCLASSIFIED**	19. SECURITY CLASSIFICATION OF ABSTRACT **UNCLASSIFIED**	20. LIMITATION OF ABSTRACT **UL**

NSN 7540-01-280-5500 **Standard Form 298**
(Rev.2-89)
Prescribed by ANSI Std. 239-18

298-102

ARMY RESEARCH OFFICE CONTRACT/GRANT NUMBER: DAAD19-02-1-0363

FINAL REPORT
(08/15/02 – 08/31/03)

Alloys-by-Design Strategies Using Stochastic Multi-Objective Optimization

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1. Foreword

We proposed to use and adapt an advanced semi-stochastic algorithm for constrained multi-objective optimization and combine it with experimental testing and verification to determine optimum concentrations of alloying elements in heat-resistant and corrosion-resistant H-Series austenitic stainless steel alloys that will simultaneously maximize a number of alloy's mechanical and corrosion properties. The proposed research was expected to result in a rigorous tool for the design of high-strength and high-temperature steels and other types of alloys that are unattainable by any means existing at the present time. Such a materials design tool was expected to reduce or minimize the need for the addition of expensive elements such as Cr, Ni, Co, Nb, Ti, V, etc. and still obtain the optimum properties of the alloy. The proposed program is also consistent with the objectives of the BAA solicitation in that it directly addresses: (a) new class of alloys for high-temperature strength, corrosion, and thermal fatigue resistance; (b) application of combinatorial methods for rapid screening of materials for industrial applications and/or materials property optimization; and (c) acquisition of thermophysical property data needed for materials processing and industrial application, a clear path to solution of major problems in modeling, process simulation, and control in design of new materials. Proof-of-the concept objectives were met during the August 15, 2002 – August 31, 2003 period of this grant as it is described in more detail in this final report.

2. Table of Contents

3. List of Appendices, Illustrations and Tables

4. Statement of the Problem Studied

We proposed to use and adapt an advanced semi-stochastic algorithm for constrained multi-objective optimization and combine it with experimental testing and verification to determine optimum concentrations of alloying elements in heat-resistant and corrosion-resistant H-Series austenitic stainless steel alloys that will simultaneously maximize a number of alloy's mechanical and corrosion properties. Such a tool is expected to minimize the need for the addition of expensive elements such as Cr, Ni, Co, Nb, Ti, V, etc. and still obtain the optimum properties needed to design the components. To reduce the computing time significantly, and to assure that globally optimal solutions will be found, we propose to develop a multi-level and multi-objective constrained optimization methodology that is a modified version of a method of Indirect Optimization based upon Self-Organization (IOSO) and evolutionary simulation principles. The optimization algorithm allows for a finite number of non-reactive ingredients in the alloy to be optimized so that a finite number of physical properties of the alloy is either minimized or maximized, while satisfying a finite number of equality and inequality constraints. The multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. Both weighted linear combination of several objectives and true multi-objective formulation options creating Pareto fronts will be utilized in the algorithm.

The main benefits of this algorithm are its outstanding reliability in avoiding local minimums, its computational speed, and a significantly reduced number of required experimentally evaluated alloy samples as compared to more traditional gradient-based and genetic optimization algorithms. Furthermore, the self-adapting response surface formulation used in this project allows for incorporation of realistic non-smooth variations of experimentally obtained data and for accurate interpolation of such data. We proposed to use a combination of analysis and experimental tools with different levels of sophistication in the multi-objective optimization of complex alloy systems. Experimentally preparing samples of those alloys and testing them will verify the Fe-Cr-Ni alloy compositions determined from the multi-objective optimization. At the same time, the proposed approach is expected to minimize the number of required time-consuming experimental evaluations. This optimization methodology is also scalable and capable of handling dozens of design variables, dozens of objectives and constraints, and performing on commodity processors.

The proposed research, although applicable to optimization of composition of arbitrary alloys, will in this project result in a rigorous tool for the design of high-strength corrosion-resistant H-Series steels unattainable by any means existing at the present time. The final outcome of the project will be the ability of H-Series stainless steel producers and users to predict either the alloy compositions for desired set of thermo-mechanical properties.

5. Summary of the Most Important Results

5.1 Background

Alloy design for critical aero-engine components such as turbine blades and discs is a difficult, time-consuming and expensive process. The development period prior to application in an engine is typically of the order of ten years. Airframe manufacturers usually announce a new design only five years prior to flight certification. This leaves the engine designers only half the current period necessary for materials development.

Nickel-based super-alloys are essentially mixtures of γ' precipitates ($L1_2$ structure) in a disordered γ (cubic-close packed structure) matrix. Despite decades of research on the γ/γ' nickel base super-alloy system, new alloys have in the past been investigated by making as many as hundreds of different variants. Each of these has to be cast or made into powder form, thermo-mechanically processed, assessed for the presence of deleterious phases and for processability, and tested on a laboratory scale. There is typically a further stage of optimization based on personal experience and intuition before a small selection of alloys is finally tested to commercial standards. Thus, the development of new nickel alloys for aero-engine applications is a difficult task, frequently achieved by trial and experience. Predictive modeling and mathematical optimization, at any stage of this empirical alloy design procedure, would obviously reduce the cost and the time involved in the development of new materials, as well as produce alloys with superior performance.

The purpose of the proposed research was to enable a significant proportion of the development procedure to be done by computation by using the power of true mathematical evolutionary optimization techniques in their direct and inverse modes.

5.1.1 The Cambridge University Effort

Probably the most prominent center for research activity in certain aspects of predictive modeling and regression analysis in super-alloys is at Cambridge University in the U.K. (Jones, MacKay and Bhadeshia, 1995; Fujii, MacKay and Bhadeshia, 1996; Jones and MacKay, 1996; Schooling and Reed, 1996; MacKay, 1997; Narayan et al., 1998; Singh et al., 1998; Yoshitake et al., 1998). Their approach is to use artificial neural network logic for a non-linear regression analysis where the input data, x_j, are multiplied by weights, but the sum of all these products forms the argument of a hyperbolic tangent. The output, *y,* is therefore a non-linear function of x_j, the function usually chosen being the hyperbolic tangent because of its flexibility. Altering the weights can vary the exact shape of the hyperbolic tangent. Further degrees of non-linearity can be introduced by combining several of these hyperbolic tangents, so that the neural network method is able to capture almost arbitrarily non-linear relationships. For example, it is well known that the effect of chromium on the microstructure of steels is quite different at large concentrations than in dilute alloys. Ordinary regression analysis cannot cope with such changes in the form of relationships.

Using artificial neural networks, the Cambridge group has successfully addressed solid solution strengthening, tensile properties, fatigue, creep, lattice misfit in the context of nickel-base super-alloys, and has applied the method to other materials and processes. A large number of quantitative models have been produced by the Cambridge group, dealing with the microstructure and mechanical properties of nickel-base super-alloys. This is the first time it has become possible to estimate properties as complex as the fatigue crack growth rate as a function of a very large number of variables. The models have been tested successfully against the known principles of physical metallurgy. They have been used already, both in reducing the scale of experimental programs and in identifying regimes where experiments are essential.

5.1.2 The Artificial Neural Network

Many mechanical properties are so complex in their dependence on material characteristics that there are no theories available to make quantitative predictions of the kind necessary in engineering design. The neural network method is ideal in such circumstances since it thrives in complexity, and when combined with experience from physical metallurgy, can be enormously useful both in the design of new materials and in the definition of critical experiments.

Neural networks are parameterized non-linear models used for empirical regression and classification modeling. Stated simply, this represents a method for the quantitative recognition of patterns in data, without any *a priori* specification of the nature of the relationship between the input and output variables. They can model relationships of almost arbitrary complexity.

The outcome of neural network training is a set of coefficients (called weights) and a specification of the functions that in combination with the weights relate the input to the output. The training process involves a search for the optimum non-linear relationship between the inputs and the outputs and is computer intensive. Once the network is trained, estimation of the outputs for any given inputs is very rapid.

There are methods, such as that of MacKay (1997), which implement a Bayesian framework on the neural network. This helps in the determination of the relevance of individual inputs. Furthermore, the error bars then depend on the specific position in input space, reducing the dangers of extrapolation and interpolation. The Cambridge group has found that this method is capable of revealing interesting metallurgical trends.

The yield and ultimate tensile strength of nickel-base super-alloys with γ/γ' microstructures has been modeled (Jones and MacKay, 1996; Jones, MacKay and Bhadeshia, 1995) using the neural network method, as a function of the Ni, Cr, Co, Mo, W, Ta, Nb, Al, Ti, Fe, Mn, Si, C, B, and Zr concentrations, and of the test temperature. The analysis was based on data selected from the published literature. The trained models were subjected to a variety of metallurgical tests. As expected, the test temperature (in the range 25-1100 °C) was found to be the most significant variable influencing the tensile properties, both via the temperature dependence of strengthening mechanisms and due to variations in the γ' fraction with temperature. Since precipitation hardening is a dominant strengthening mechanism, it was encouraging that the network recognized Ti, Al and Nb to be key factors controlling the strength. The physical significance of the neural network was apparent in all the interrogations we performed.

A further revelation from the neural network analysis came from the error estimates, which demonstrated clearly that there are great uncertainties in the experimental data on the effect of large concentrations of molybdenum on the tensile properties. This has identified a region where careful experiments are needed since molybdenum is known to have a large influence on the γ/γ' lattice misfit.

The Cambridge group methodology for tensile properties has already been exploited in Rolls-Royce to reduce the number of variants involved in experimental alloy design programs.

The creep rupture life of nickel base super-alloys has been modeled as a function of 42 variables including Cr, Co, C, Si, Mn, P, S, Mo, Cu, Ti, Al, B, N, Nb, Ta, Zr, Fe, W, V, Hf, Re, Mg, La and ThO_2 (Fujii et al., 1998). Other variables included four heat treatment steps (characterized by temperature, duration and cooling rate), the sample shape and the solidification method. The results have been interpreted using physical metallurgy principles where this is possible, and the model is currently being used in the Technology Foresight Program at Cambridge University.

The treatment of iron-base super-alloys using both neural network and physical modeling is described by Badmos, Bhadeshia and MacKay (1998) and by Badmos and Bhadeshia (1997). A description of the modeling of constitutive relations obtained by torsion testing is offered by Narayan et al., (1998). The modeling of steel plate processing using more than 100 variables is given by Singh et al. (1998). A lot of the work and data are available from the materials algorithms project website *http: / /www.msm cam. ac. uk/map/mapmain. html*

Neural network models in many ways mimic human experience and are capable of learning or being trained to recognize the correct science rather than nonsensical trends. Unlike human experience, these models can be transferred readily between generations and steadily developed to make design tools of lasting value. These models also impose a discipline on the digital storage of valuable experimental data, which may otherwise be lost with the passage of time.

A potential difficulty with the use of regression methods is the possibility of over-fitting data. For example, it is possible to produce a neural network model for a completely random set of data. To avoid this difficulty, the experimental data can be divided into two sets, a *training* dataset and a *test* dataset. The model is produced using only the training data. The test data are then used to check that the model behaves itself when presented with previously unseen data.

In addition, artificial neural networks, once fully trained, are very efficient and accurate interpolating algorithms for any multi-parameter function. However, this does not mean that the neural networks are automatically efficient and accurate search algorithms or extrapolation algorithms. These, they are not.

Therefore, it is important to understand a need for a mathematically sound multi-objective stochastic optimization algorithms that are capable of finding the global minimum and confidently search outside a given initial data base.

5.1.3 Multi-objective Optimization: Background

This proposal deals with the industry-wide need for improving material property performance for the applications that they are currently used for and to increase their upper use temperature, strength, and corrosion resistance. The proposed project takes the new approach of using stochastic optimization algorithm for optimizing alloy properties with a minimum number of experimental evaluations of the candidate alloys. This approach has the potential of identifying new compositions that cannot be identified without carrying out an unacceptably large number of experiments. Furthermore, this approach has the potential for creating and designing alloys for each application, thereby maximizing their utilization at reduced cost.

The key to the success of the proposed research is the robustness, accuracy, and efficiency of the multi-objective constrained optimization algorithm. There are only a few commercially available general-purpose optimization software packages. Currently, the most popular commercially available general-purpose optimization software in the United States is iSIGHT (1995). However, these software packages predominantly use a variety of standard gradient-based optimization algorithms which are known to be unreliable because of their tendency to terminate in the nearest feasible minimum instead of finding a global optimum. Moreover, these optimizers can perform only optimization of a weighted linear combination of objective functions. This formulation does not provide a true multi-objective optimization capability, that is, each individual objective is not fully maximized. Furthermore, these optimizers require an extremely large number of objective function (mechanical and corrosion properties of alloys) evaluations, which makes the total number of experimental evaluations unacceptably large.

The U.S. domestic industry is most probably aware of these drawbacks of the commercially available optimization software. Some of them are also becoming aware of the neural network approach to alloy design as practiced at Cambridge University. However, for the most part they are not aware of the latest developments in the area of stochastic

truly multi-objective constrained optimization since these methods have not been commercialized and have not been demonstrated in this field of application.

Our proposed research is based on the use and a special adaptation of a new stochastic optimization algorithm specifically for the task of optimizing properties of alloys while minimizing the number of experimental evaluations of the candidate alloys.

With the continuing growth of computing resources available, the attention of design engineers has been rapidly shifting from the use of repetitive computational analysis, personal experience, and intuition towards a reliable and economical mathematically based optimization algorithms. This trend has exposed the practical limitations of traditional gradient based optimization approaches that easily terminate in a local minimum, can usually produce only single-objective optimized solutions, and require that the objective function satisfies continuity and derivability conditions. These facts, together with the growing need for the multi-disciplinary and multi-objective approach to design with a large number of design variables, resulted in an increased interest in the use of various versions of hybrid (Dulikravich et al., 1999; Martin and Dulikravich, 2001), semi-stochastic (Poloni et al., 1999; Dennis et al., 2000; Dennis and Dulikravich, 2001), and stochastic (Egorov, 1992a, 1993; Egorov and Kretinin, 1993, 1996; Egorov et al., 1999b; Dulikravich et al., 2003; Dennis et al. 2003a; 2003b) optimization algorithms. It should be pointed out that including more objectives in the optimization process often has similar effects on the overall optimization effort required as including more constraints especially if these constraints are incorporated as penalty functions.

Multi-objective optimization algorithms based on a genetic algorithm have been successfully applied in a number of engineering disciplines. However, for a large number of design variables and objective functions that need to be extremized simultaneously, this approach becomes progressively too time consuming and unreliable for practical applications in industry.

The *multi*-objective optimization problem maximizes a vector of n objective functions

$$max \; F_i(\overline{X}) \qquad \text{for } i = 1, \ldots n \tag{1}$$

subject to a vector of inequality constraints

$$g_j(\overline{X}) \leq 0 \qquad \text{for } j = 1, \ldots m \tag{2}$$

and a vector of equality constraints

$$h_q(\overline{X}) = 0 \qquad \text{for } q = 1, \ldots k \tag{3}$$

In general, the solution of this problem is not unique. With the introduction of the Pareto dominance concept the possible solutions are divided in two subgroups: the *dominated* and the *non-dominated*. The solutions belonging to the second group are the "efficient" solutions, that is, the ones for which it is not possible to improve any individual objective without deteriorating the values of at least some of the remaining objectives.

In formal terms, in case of a maximization problem, it is possible to write that the solution $\overline{X}$ dominates the solution $\overline{Y}$ if the following relation is true.

$$\overline{X} >_p \overline{Y} \Leftrightarrow (\forall i F_i(\overline{X}) \geq F_i(\overline{Y})) \cap (\exists j : F_j(\overline{X}) > F_j(\overline{Y})) \tag{4}$$

Classical gradient-based optimization algorithms are capable, under strict continuity and derivability hypotheses, of finding the optimal value only in the case of a single objective. For these algorithms, the problem of finding the group of non-dominated solutions (the Pareto front) is reduced to several single objective optimizations where the objective becomes a weighted combination of the objectives called utility function.

The proposed project takes a new approach of using stochastic optimization algorithm for optimizing alloy properties with minimum number of experimental evaluations of the candidate alloys. The proposed approach has the potential of identifying new compositions that cannot be identified without carrying out thousands of experiments. Furthermore, the approach has the potential for creating and designing alloys for each application, thereby maximizing their utilization at reduced cost.

The key to the success of the proposed research is the robustness, accuracy, and efficiency of the proposed multi-objective constrained optimization algorithm. There are only a few commercially available general-purpose optimization software packages. They all use almost exclusively a variety of standard gradient-based optimization algorithms, which are known to be unreliable because of their tendency to terminate in the nearest feasible minimum instead of finding a global optimum. Moreover, these optimizers can perform only optimization of a weighted linear combination of objective functions. This formulation does not provide a true multi-objective optimization capability, that is, each individual objective is not fully maximized. These optimizers require an extremely large number of objective function (mechanical and corrosion properties of alloys) evaluations, which makes the total number of experimental evaluations unacceptably large.

However, semi-stochastic truly multi-objective constrained optimization algorithms have not been commercialized yet and have not been demonstrated in this field of application. The proposed research is based on the use and a special adaptation of a new stochastic optimization algorithm specifically for the task of optimizing properties of alloys while minimizing the number of experimental evaluations of the candidate alloys. The proposed multi-objective optimization algorithm is of a semi-stochastic type incorporating certain aspects of a selective search on a continuously updated multi-dimensional response surface. Both weighted linear combination of several objectives and true multi-objective formulation options creating Pareto fronts are incorporated in the algorithm. The main benefits of this algorithm are its outstanding reliability in avoiding local minimums, its computational speed, and a significantly reduced number of required experimentally evaluated alloy samples as compared to more traditional semi-stochastic optimizers like genetic algorithms. Furthermore, the self-adapting response surface formulation used in this project allows for incorporation of realistic non-smooth variations of experimentally obtained data and allows for accurate interpolation of such data.

5.1.4 Response Surface and Self-Organization Concepts

Our approach to the MDO concept is based on the widespread application of response surface technique, based upon the original approximation concept, within the frameworks of which we adaptively use global and middle-range multi-point approximation. One of the advantages of the proposed approach is the possibility of ensuring good approximating capabilities using minimum amount of available information. This possibility is based on self-organization and evolutionary modeling concepts (Egorov, 1998). During the approximation, the approximation function structure is being evolutionarily changed, so that it allows successful approximation of the optimized functions and constraints having sufficiently complicated topology. The obtained approximation functions can be used by multi-level MDO procedures with the adaptive change of simulation level within both a single and multiple disciplines of object analysis, and also for the solution of their interaction problems.

With reference to a particular problem of the creation of an alloy with desirable properties, there will inevitably arise a problem of constraints that need to be specified on the objective functions. These constraints are absent in a more general multi-objective optimization statement. Such objective constraints should be set by the user (expert) and could be allowed to vary during the solution process. For example, a minimum acceptable value for the Young's modulus of elasticity could be specified as an inequality constraint. Or, a maximum acceptable percentage for each of the most expensive ingredients in the alloy could be specified as a cost objective constraint. Also, the total acceptable manufacturing cost of an alloy could be specified as an equality constraint.

The problem of search for Pareto - optimum solutions set in the multi-objective optimization while varying chemical composition of an alloy would be an unacceptably labor-intensive process. This is because of an extremely large number of alloy compositions that would need to be created and because several of the properties of each of these alloys would have to be evaluated experimentally. In this case, we can speak only about the creation of some rather extensive database including the information on various properties of alloys for various combinations of a chemical structure. Such a database could be used for the solution of particular problems aimed at the creation of alloys with desirable properties.

Instead, we propose to use IOSO multi-objective optimization (Egorov et al., 1999a, 1999b; Dennis et al., 2000a) to determine alloy compositions offering optimum properties of alloys.

Unfortunately, such problems, as a rule, are difficult to formalize at the initial stage, since the user does not know initially what values of some objectives could be reached and how the remaining objectives will vary. That is, the user has very little if any *a priori* knowledge of objective function space topology.

For example, for the solution of an actual problem in the car industry with 6 variables we needed nearly 60 experiments when using a basic IOSO algorithm. However, for optimization of the classical Rosenbrock test function, having only 2 variables, it was necessary to perform almost 300 objective function evaluations. Hence, it is very difficult to predict the number of experiments required in the optimization application proposed here.

Therefore, it seems, that such problems of optimization can be solved only in an interactive mode, when the user during the solution can change both objective constraints and objective functions. Actually, in this case one can speak about optimally controlled experiments. Let us consider several different scenarios for the solution of optimization problem for these conditions.

The first approach is to perform a general multi-objective optimization of the material properties.

Within the framework of this strategy we are to solve the multi-objective optimization problem (to find the Pareto set) using the general IOSO algorithm. This strategy is the most accurate, but it requires a very large number of experiments.

The second approach is an interactive step-by-step optimization of the material properties. The first step of this strategy is to create an initial plan of experiments. This involves formulation of a single (hybrid) optimization objective by the user. This objective may be the convolution of particular objectives with different weight coefficients assigned to each of them. Then, one optimization step is needed to minimize this composite objective. The result of this strategy is the single, not Pareto-set, solution. However, during such relatively efficient quasi multi-objective optimization process we can accumulate the information about the particular objectives and construct progressively more accurate response surface models.

Thus, in order to develop and realize the most effective optimization strategies, both of the first and the second kind, we have to perform a thorough preliminary search for the classes of base functions that will be able to construct the most accurate response surface models.

However, the number of experiments that is necessary for true multi-objective optimization problem solution depends not only on the dimensionality of the problem (the number of ingredient species in an alloy); it also depends to a considerable degree on the topologies of the object functions.

5.1.5 Summary of IOSO Algorithm

Each iteration of IOSO consists of two steps. The first step is the creation of an approximation of the objective function(s). Each iteration in this step represents a decomposition of the initial approximation function into a set of simple approximation functions so that the final response function is a multi-level graph.

The second step is the optimization of this approximation function. This approach allows for corrective updates of the structure and the parameters of the response surface approximation. The distinctive feature of this approach is an extremely low number of trial points to initialize the algorithm.

The obtained response functions are used in the multi-level optimization while adaptively utilizing various single and multiple discipline analysis tools that differ in their level of sophistication. During the process of each iteration of IOSO, the optimization of the response function is performed only within the current search area.

This step is followed by a direct call to the mathematical analysis model or an actual experimental evaluation for the obtained point. During the IOSO operation, the information concerning the behavior of the objective function in the vicinity of the extremum is stored, and the response function is made more accurate only for this search area. While proceeding from one iteration to the next, the following steps are carried out: modification of the experiment plan; adaptive selection of current extremum search area; choice of the response function type (global or middle-range); transformation of the response function; modification of both parameters and structure of the optimization algorithms; and, if necessary, selection of new promising points within the researched area. Thus, during each iteration, a series of approximation functions for a particular objective of optimization is built. These functions differ from each other according to both structure and definition range. The subsequent optimization of these approximation functions allows us to determine a set of vectors of optimized variables.

During this work (Dulikravich, Egorov, Sikka and Muralidharan, 2003) algorithms of artificial neural networks (ANN) were used that utilized radial-basis functions modified in order to build the response surfaces. The modifications consisted in the selection of ANN parameters at the stage of their training that are based on two criteria: minimal curvature of response surface, and provision of the best predictive properties for given subset of test points $W_{best} \in W_{ini}$. Each iteration of alloy composition multi-objective optimization technique involves the following steps:

1. Building and training ANN1 for a given set of test points proceeding from the requirement $W_{best} = W_{ini}$.
2. Conducting multi-objective optimization with the use of ANN1 and obtaining a specified number of Pareto optimal solutions P_1.
3. Determining a subset of test points W_{best} that are maximally close to points P_1 in the space of variable parameters.
4. Training ANN2 proceeding from the requirement to provide the best predictive properties for obtained subset of test points $W_{best} \in W_{ini}$.
5. Conducting multi-objective optimization with the use of ANN2 and obtaining a set of Pareto-optimal solutions P_2.

In general, the database contains information on experimentally obtained alloy properties compiled from different sources and obtained under different experimental conditions. As a result, for alloys with the same chemical compositions, there can be considerable differences of measured properties. These differences can be explained as errors due to the particular conditions existing during the experiments (measurement errors), and by the effect of certain operating conditions (for example, thermal condition of alloy making). Unless operating conditions are quantified numerically, their influence is regarded as an additional chance factor. In its simplified form the methodology can be presented as the following set of actions:

1. Formulation of optimization task, that is, selection of variable parameters, definition of optimization objectives and constraints, and setting initial (preliminary) ranges of variable parameters variations.
2. Preliminary reduction of the experimental database. At this stage the points meeting optimization task statement are picked up from the database so that alloys having chemical composition outside the chosen set of variable parameters are rejected. Alloys for which there is no data for at least one optimization objective are rejected. In addition, alloys with chemical compositions outside the set range of variable parameters are also rejected.
3. Final reduction of the experimental database. Since accuracy of the building of response surfaces substantially depends on uniformity of distribution of variable parameters in the surveyed area, rejection of experimental data points falling outside of the universal set is performed. At the end of this stage, a final range of variable parameters for optimization is set.
4. Execution of multi-objective optimization resulting in a specified number of Pareto optimal solutions.
5. Analysis of optimization results.
6. Carrying out an experiment to obtain a set of Pareto optimal alloy compositions (or a certain subset) and analysis of the results obtained.
7. Change of optimization problem statement (number of simultaneous objectives and constraints, the set and range of variable parameters), and returning to step 2.

8. Modification of database and returning to step 4.
9. Stop

5.2 Initial (universal) experimental database

For this particular case, the initial data represented a database containing information on 201 experimentally tested alloys. The data are contained in the file ***ini_data.xls***. A preliminary analysis of data has shown that for certain alloys there is no complete information on alloy chemical composition. Such alloys were excluded from further analysis. Besides, some chemical elements (***V, Bi, Se, Zr, Sb, Cd*)** were present in a very small number of alloys, which makes it impossible to assess their effect proceeding from information in this database. Such alloys were also excluded from further analysis. The remaining database had 176 alloys (file ***first.xls***).

At the next stage, an evaluation of uniformity of distribution of the percentage values of different elements in the existing range was made. It turned out that certain alloys had percentages differing very strongly from the universal set. As an example Fig.1 presents distribution of the percentage of sulfur in the alloys of the reduced database. The alloy No.67 had percentage of sulfur exceeding average value by some 10 times. Such alloys were excluded from further analysis. The capacity of the remaining database was 158 alloys (the file ***second.xls***).

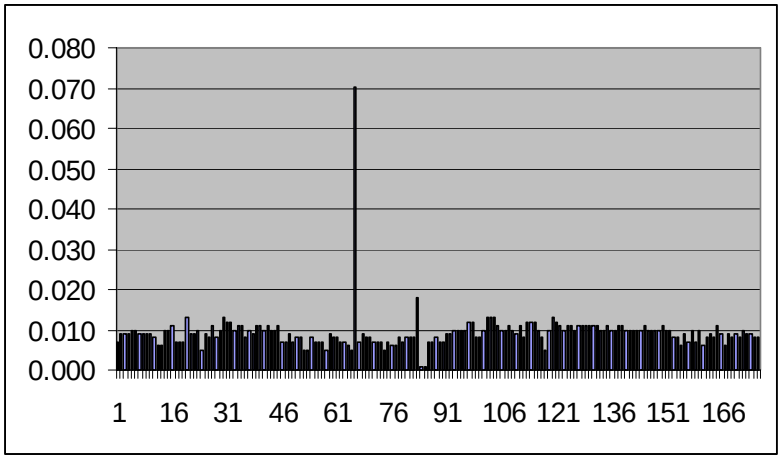


Fig. 1. Distribution of percentage of sulfur (S) in experimental database for steel alloys.

5.2.1 Variable parameters

In this problem the percentages of the following 17 elements were taken as independent variables:
C, S, P, Cr, Ni, Mn, Si, Cu, Mo, Pb, Co, Cb, W, Sn, Al, Zn, Ti.
The ranges of these elements were set as follows. First, minimum and maximum values for existing set of experimental data ($Exp\_min_i, Exp\_max_i,\ i = \overline{1,17}$) were defined. Then, new minimum and maximum values for each of the 17 elements were obtained according to the following simple dependencies:
($Min_i = 0.9 \cdot Exp\_min_i, Max_i = 1.1 \cdot Exp\_max_i,\ i = \overline{1,17}$). The existing ranges are given in Table 1.

Table 1. Ranges of variation of 17 independent variables (chemical elements in the steel alloy)

	C	S	P	Cr	Ni	Mn	Si	Cu	Mo
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074	0.016	0.000
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150	0.165	0.132

	Pb	Co	Cb	W	Sn	Al	Zn	Ti
min	0.001	0.000	0.000	0.000	0.000	0.001	0.001	0.000
max	0.006	0.319	1.390	0.484	0.007	0.075	0.015	0.198

The following parameters were used as optimization objectives:

- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

Under the research the solution of a three-objectives optimization problem and a series of two-objectives problems were accomplished when one of the considered parameters was constrained.

5.2.2 Simultaneous optimization of three objectives for alloys having 17 chemical elements

During the first stage, the problem of simultaneously optimizing three objectives was solved with 100 points of Pareto optimal solutions. The results are given in the file ***task1.xls*** *in* ***Appendix 1***. Figure 2 presents obtained Pareto optimal solutions in objectives' space (PSI – HOURS). Analysis of this figure allows us to extract an area of admissible combinations of different optimization objectives. It can be seen that results are distributed in the admissible part of the objectives' space quite uniformly. Such a distribution offers a possibility for a significant improvement of accuracy of response surfaces on condition that the experiments will be carried out at the obtained Pareto optimal points. In principle, the first iteration of the process of alloy chemical composition optimization by several objectives could be regarded as completed. Then, in accordance with the elaborated technique, it is necessary to conduct experiments at the obtained Pareto optimal points, evaluate accuracy of prediction of values of partial optimization criteria, and either complete the process or perform another iteration.

However, such a strategy seems very difficult to implement for a researcher who knows his tasks more accurately. It can be seen that the ranges of variation of optimization objectives for obtained Pareto set are very wide. At the same time, if a researcher can formulate the problem more specifically (for example, by setting constraints on the objectives) the volume of experimental work can be substantially reduced.

Figure 3 presents interdependence of the chosen optimization objectives built on the obtained set of Pareto optimal solutions. Analysis of these figures shows that the increase of temperature, for instance, leads to the decrease of compromise possibilities between PSI and HOURS. Hence, if a researcher knows exactly in what temperature range the alloy being designed will be used, it is more economical that the problem of two-objectives optimization be solved with additional constraint for the third efficiency parameter.

Larsen-Mueller diagram (Fig. 4) has PSI on the vertical axis and the following expression on the horizontal axis (Temperature in Rankine degrees) * log(HOURS + 20). Here, logarithm is with the basis 10, while temperature is in Rankine = temperature in Fahrenheit + 460.

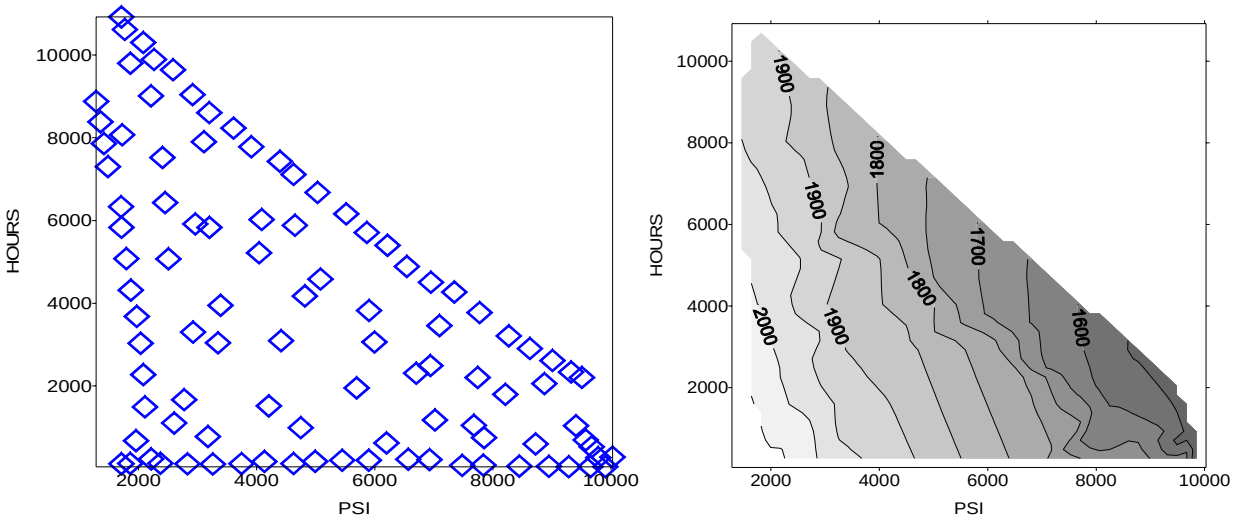


Fig.2. Time to rupture vs. strength interdependence of optimization objectives for three-objectives Pareto set.

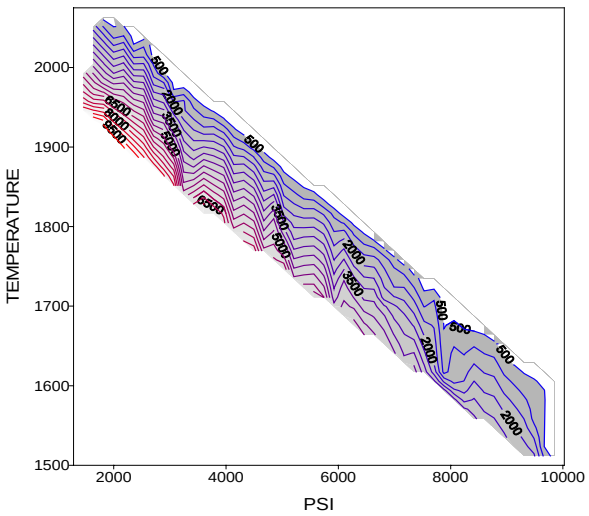


Fig.3. Temperature vs. strength iterdependence of optimization objectives for three-objectives Pareto set.

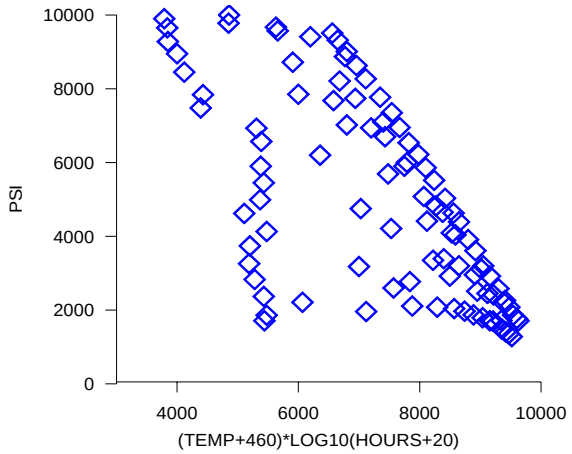


Fig. 4. Larsen-Mueller diagram for three-objectives optimization results.

5.2.3 A sequence of two-objective optimizations of alloys with 17 chemical elements

This part presents results of solution of five additional two-objectives problems in which PSI and HOURS were regarded as simultaneous objectives, and different constraints were placed on temperature:

- Problem 2. - $T \geq 1600$, number of Pareto optimal solutions is 20.
- Problem 3. - $T \geq 1800$, number of Pareto optimal solutions is 20.
- Problem 4. - $T \geq 1900$, number of Pareto optimal solutions is 20.
- Problem 5. - $T \geq 2000$, number of Pareto optimal solutions is 15.
- Problem 6. - $T \geq 2050$, number of Pareto optimal solutions is 10.

Results of solution of these problems are contained in the file ***task2-6.xls***. Some of the graphical results are presented in Figs. 5-7. Figure 5 presents obtained sets of Pareto optimal solutions in objectives space. It can be seen that maximum achievable values of PSI and HOURS, and possibilities of compromise between these parameters largely depend on temperature. For instance, the increase of minimum temperature from 1600 F to 1900 F leads to the decrease of attainable PSI by more than 50 percent. At the same time, limiting value of HOURS will not alter with the change of temperature.

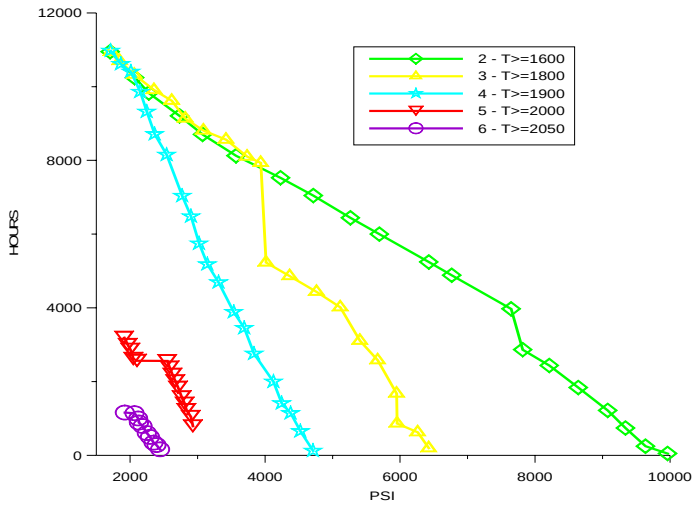


Fig. 5. Sets of Pareto optimal solutions of five problems with two-objectives.

The decrease of the number of simultaneous optimization objectives (transition from three- to two-objectives problem with constraints) leads to the decrease of the number of additional experiments needed, at the expense of both decreasing the number of Pareto optimal points and decreasing the ranges of chemical compositions.

Three-dimensional plots (Pareto surfaces) where the three coordinates are PSI, TEMP, and HOURS are given in Figures 6. Notice that since the range of Pareto-optimal points distribution is not a square, the quality of the surfaces is somewhat reduced:

Larsen-Mueller diagram for this set of cases (2-objective optimization for five temperatures) is shown in Figure 7.

We also calculated sensitivity derivatives at 7 Pareto-optimal points. These derivatives are in the "***derivatives.xls***" file. But we think, that accuracy of these evaluations is very low.

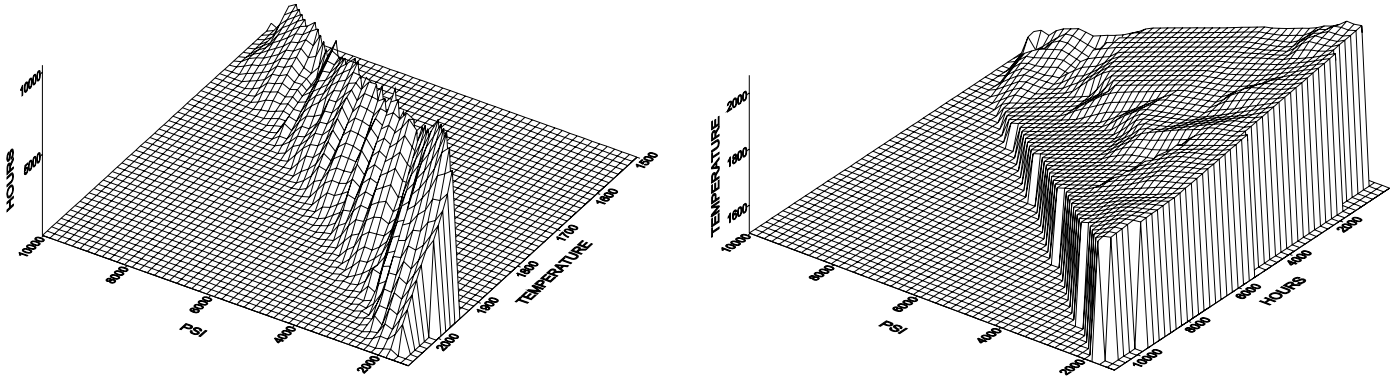


Fig. 6. Non-cumulative plots showing T=2050, T=2000, T=1900, T=1800, T=1600.

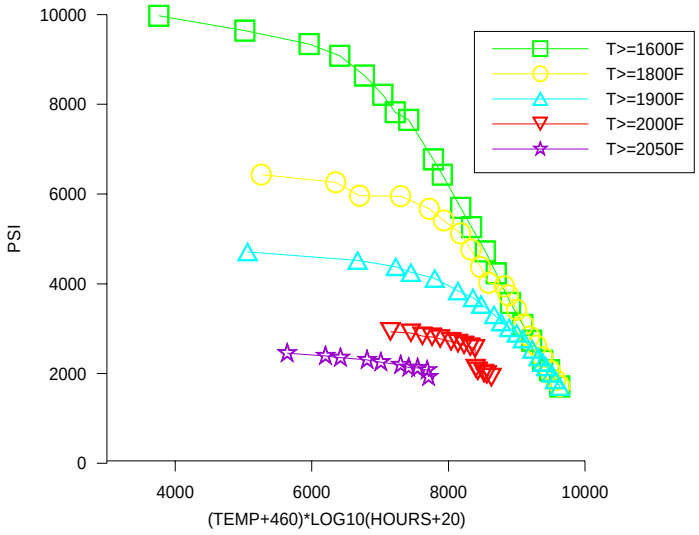


Fig. 7. Larsen-Mueller diagrams for five two-objectives optimization problems results.

Figs. 8-11 show ranges of percentages of different elements for initial set of experimental data, and for results of solution of six optimization problems. It is noteworthy that a competent analysis of results obtained can allow the specialist to soundly choose chemical compositions for which the experiment is necessary, from the viewpoint of achieving desirable values of optimization objectives and building a more accurate response surface.

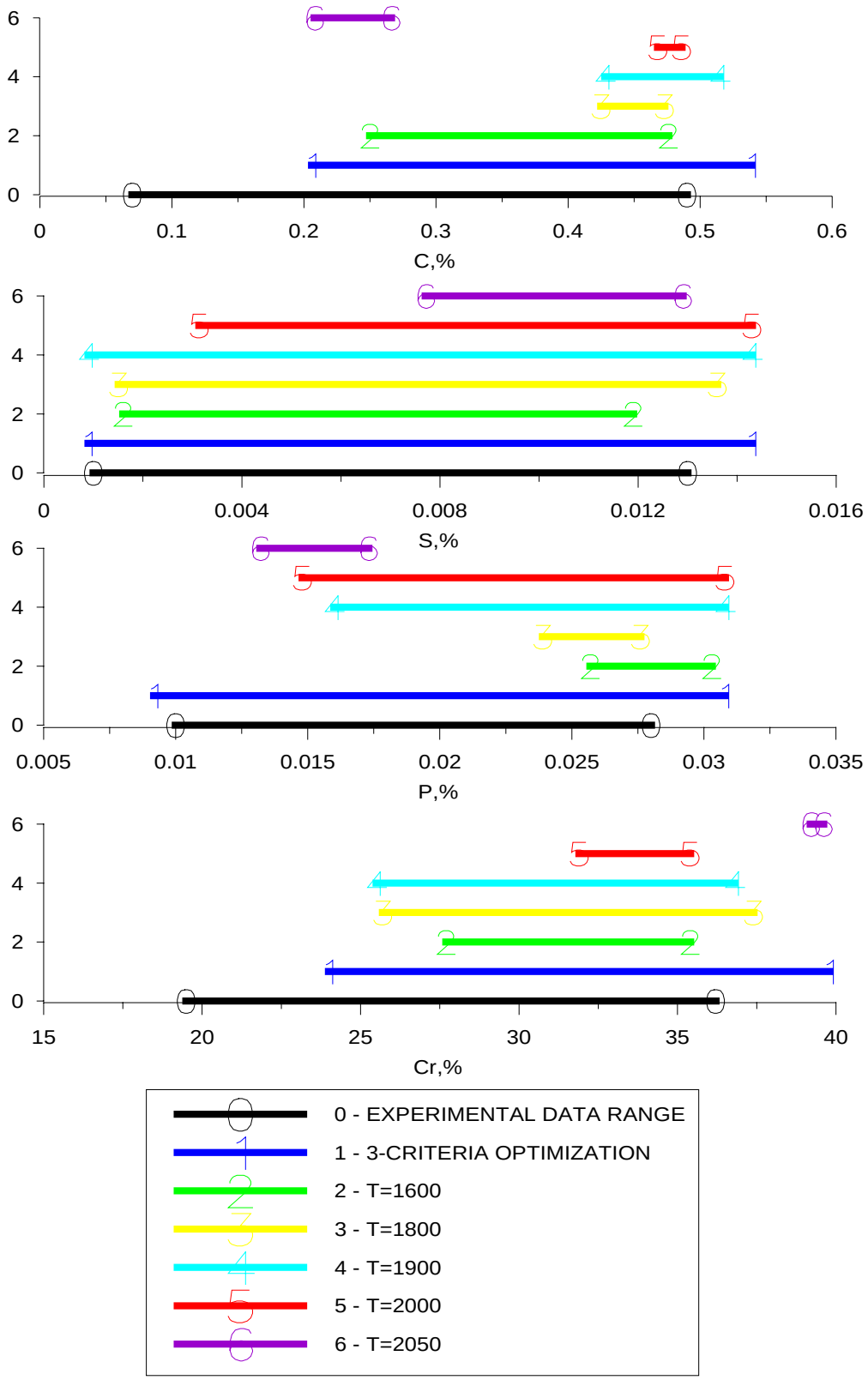


Fig. 8. Boundaries of variable parameters for two-objectives sets of Pareto optimal solutions.

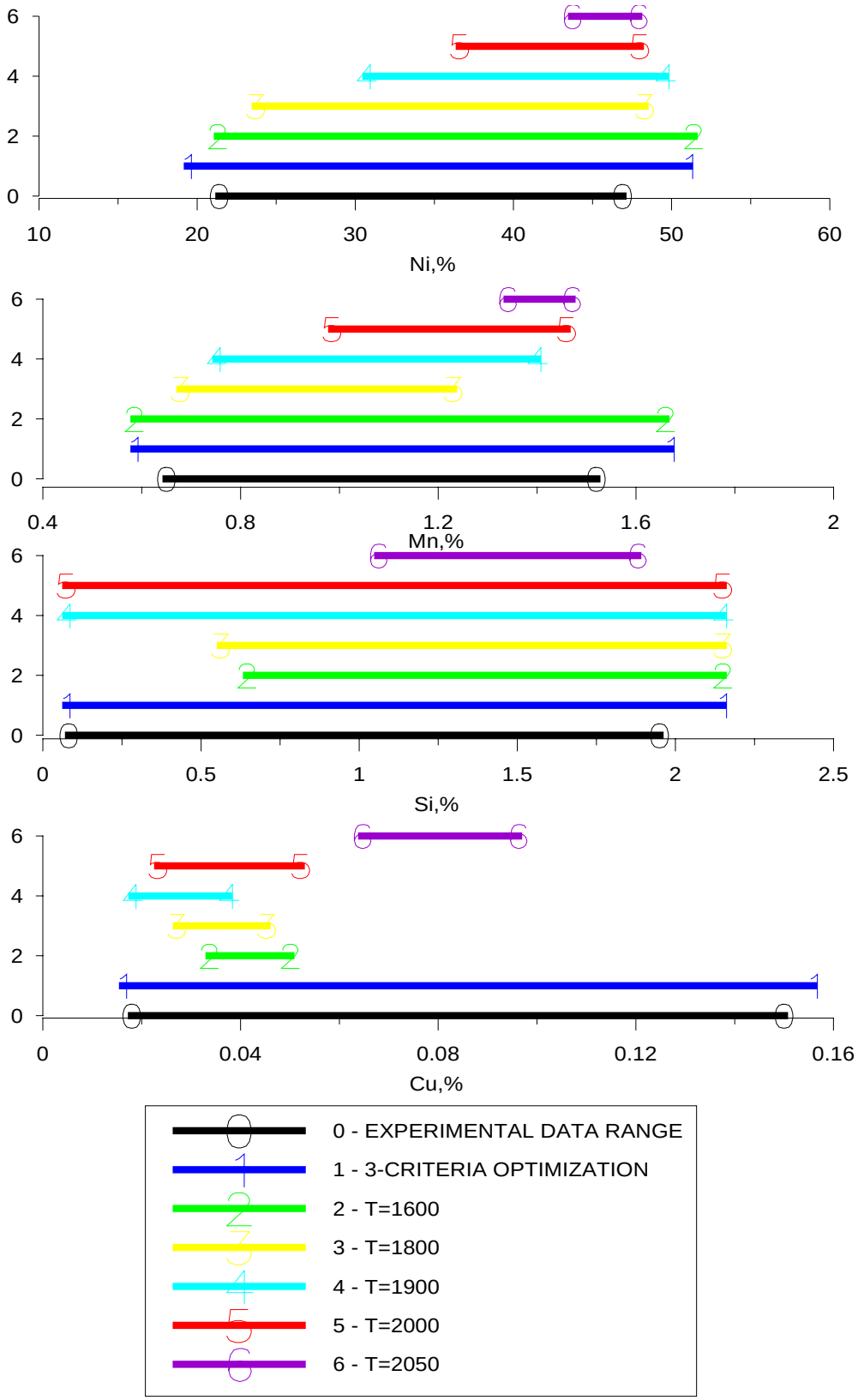


Fig. 9. Boundaries of variable parameters for sets of two-objectives Pareto optimal solutions.

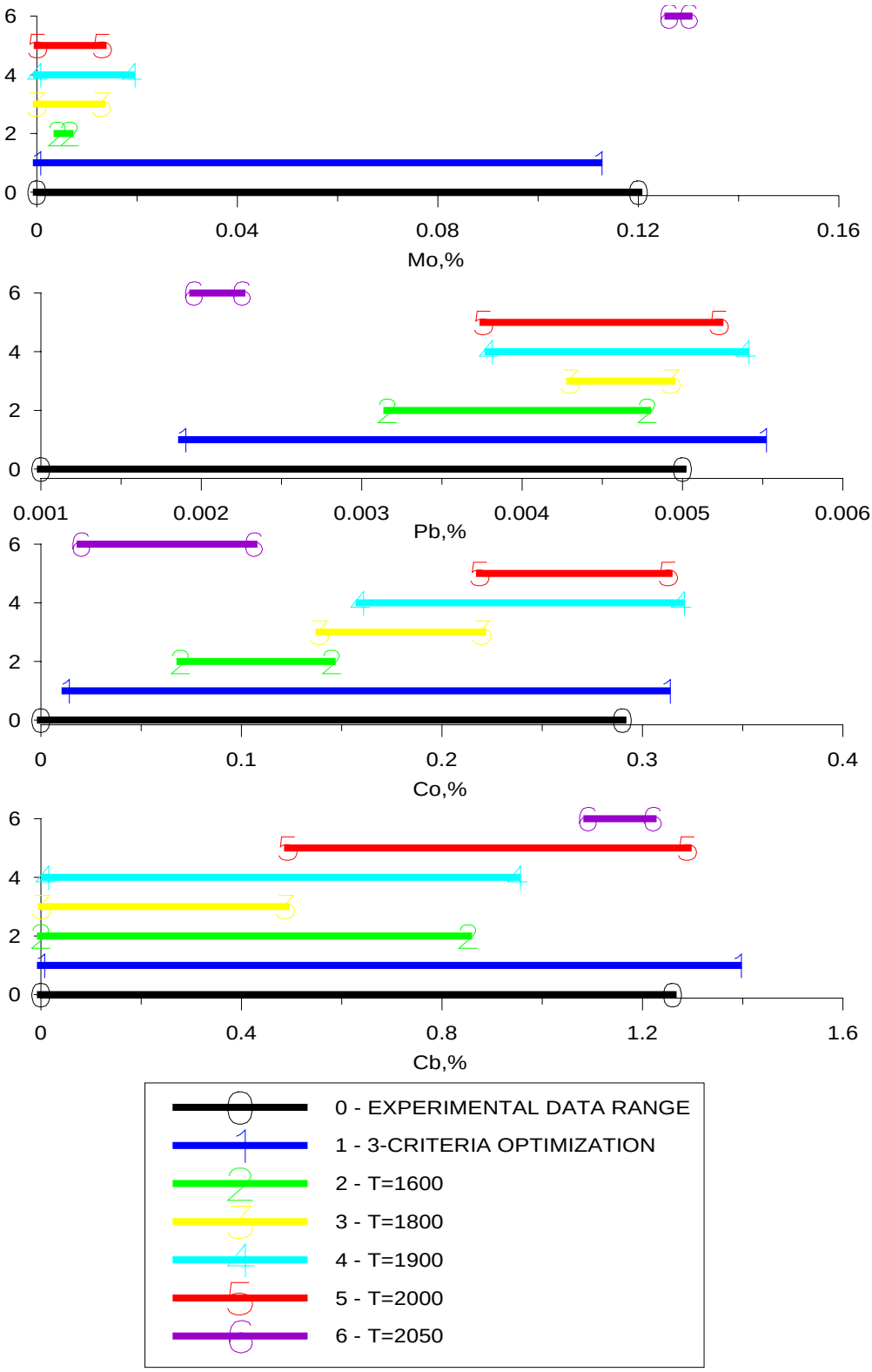


Fig. 10. Boundaries of variable parameters for sets of Pareto optimal solutions.

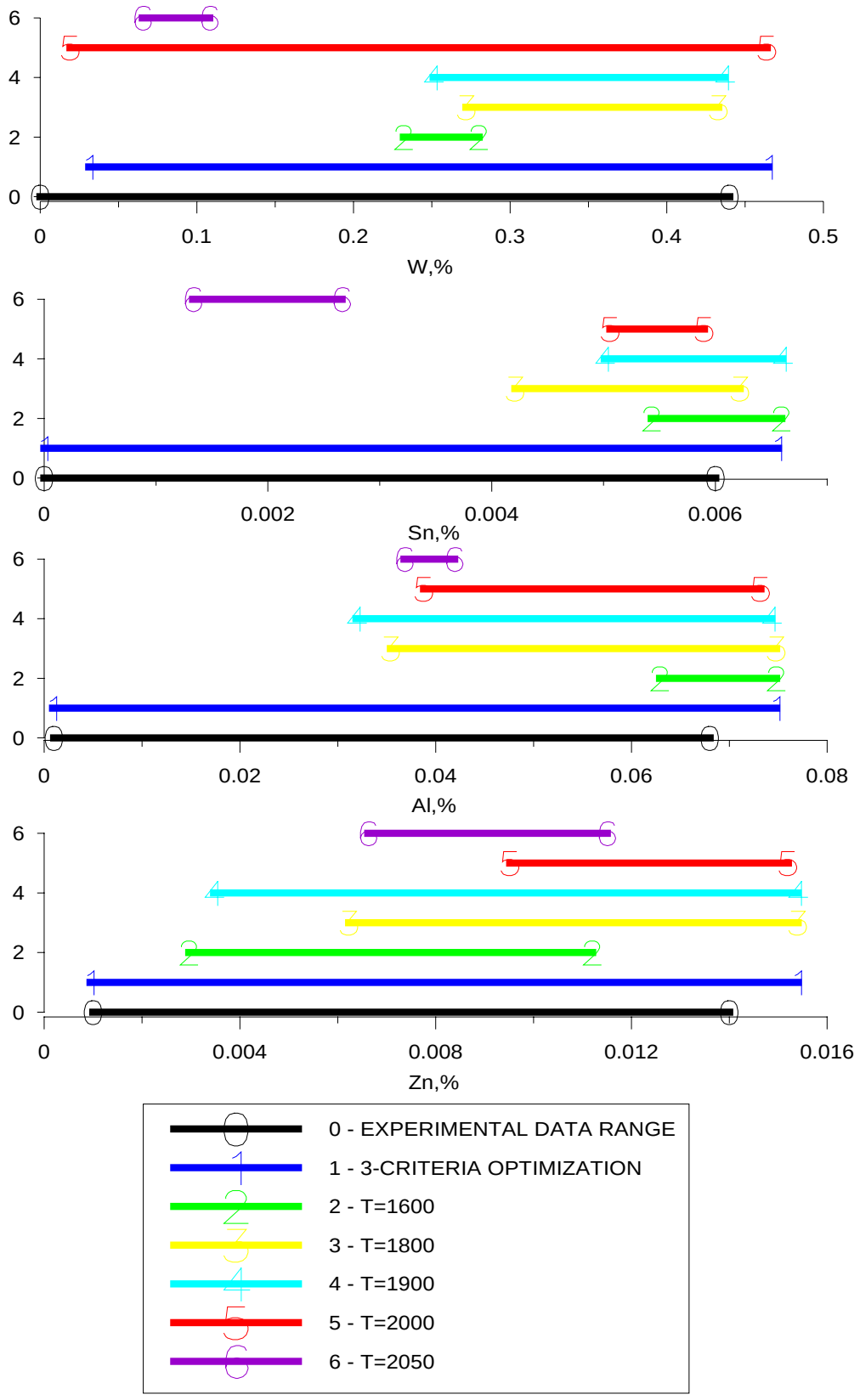


Fig. 11. Boundaries of variable parameters for sets of Pareto optimal solutions.

5.3 Optimization Results for the Cases With 9 Design Variables

We then repeated the three-objectives optimization run in which we used only the following 9 chemical elements as independent variables: ***C, Cr, Ni, Mn, Si, Mo, Cb, W, Ti***. We have followed the same steps during the optimization as when solving the problem with 17 variables. But, in this case there are differences:

Table 2. Ranges of variation of 9 independent variables (chemical elements in the steel alloy)

	C	Cr	Ni	Mn	Si	Mo	Cb	W	Ti
min	0.00	17.50	25.00	0.00	0.00	0.00	0.00	0.00	0.00
max	0.60	30.00	35.00	2.00	2.00	2.00	3.00	2.00	2.00

The main reason of accuracy of the response surface representation deterioration is that while decreasing the number of variables for the same experimental data set, we added the additional noise. For example, in the file "***distan.xls***" one can find five pairs of points that are very close in variables' space, but have drastically different values of objectives.

5.3.1 Three-criteria optimization using 9 design variables (chemical species):
*see file **v9-task1-3criteria.xls** in **Appendix 2***

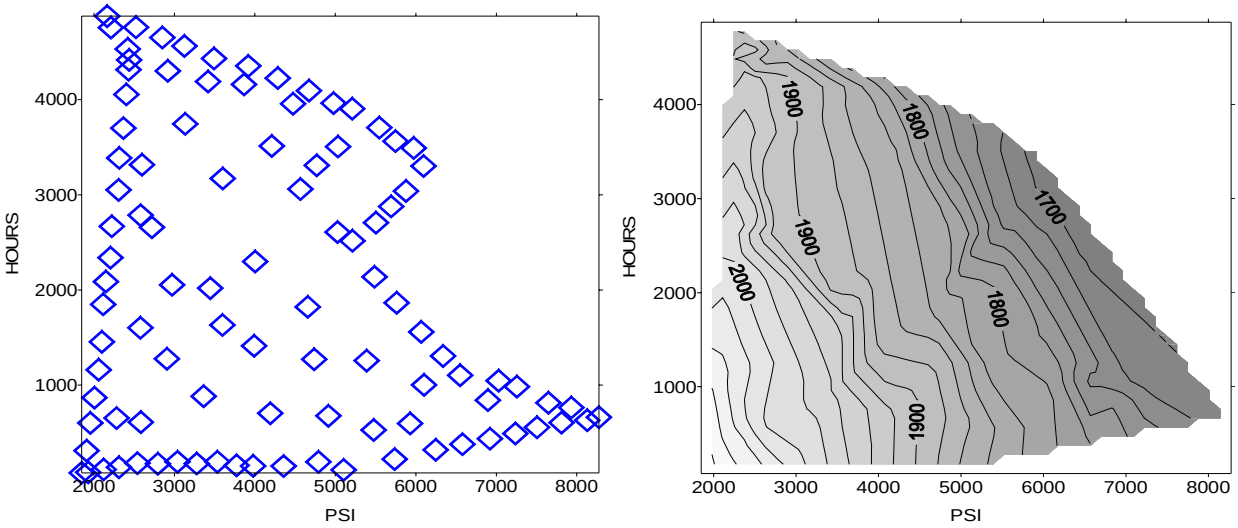


Fig.12. Distribution of points in objectives space using 9 design variables (chemical species).

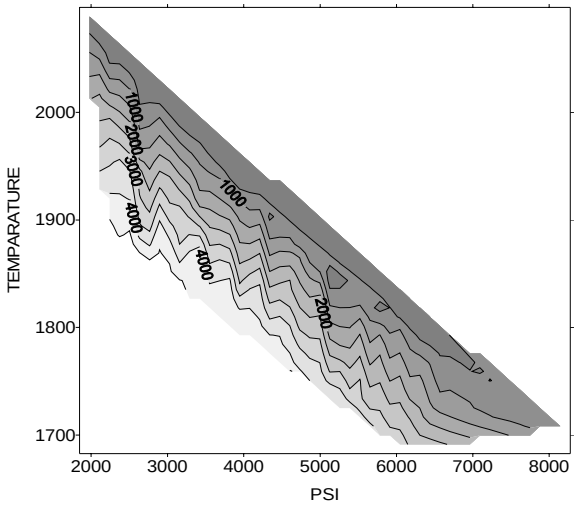


Fig. 13. Interdependence of optimization objectives for Pareto set using 9 design variables (chemical species).

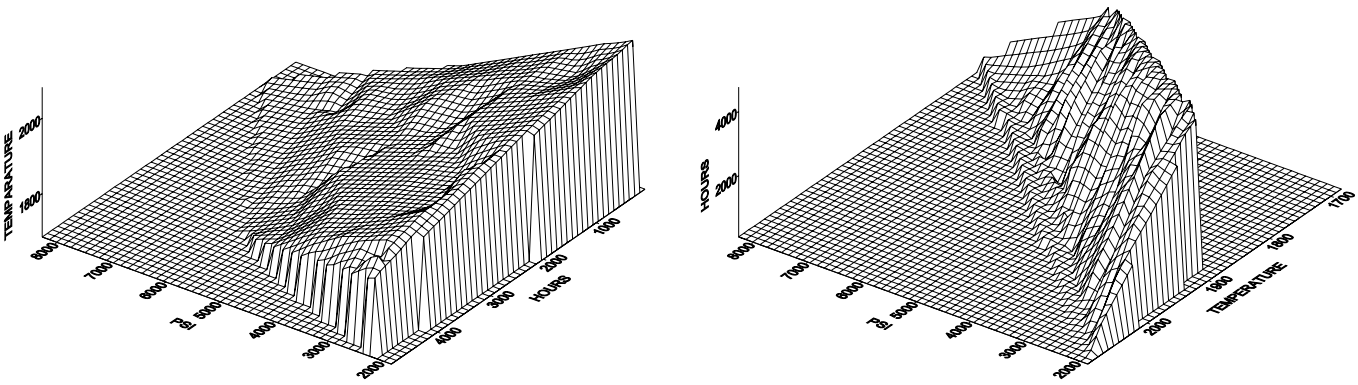


Fig.14. Pareto surfaces using 9 design variables (chemical species).

5.3.2 Two-objectives optimization using 9 design variables (tasks N2,…,N6): see file ***v9-task2-6.xls***

Analysis of the three-criteria optimization results shows that there are no solutions with temperature less or equal 1600F. Because of this, we changed the value of a constraint for the task N2. Constraint $T \geq 1600$ was replaced with $T \geq 1700$.

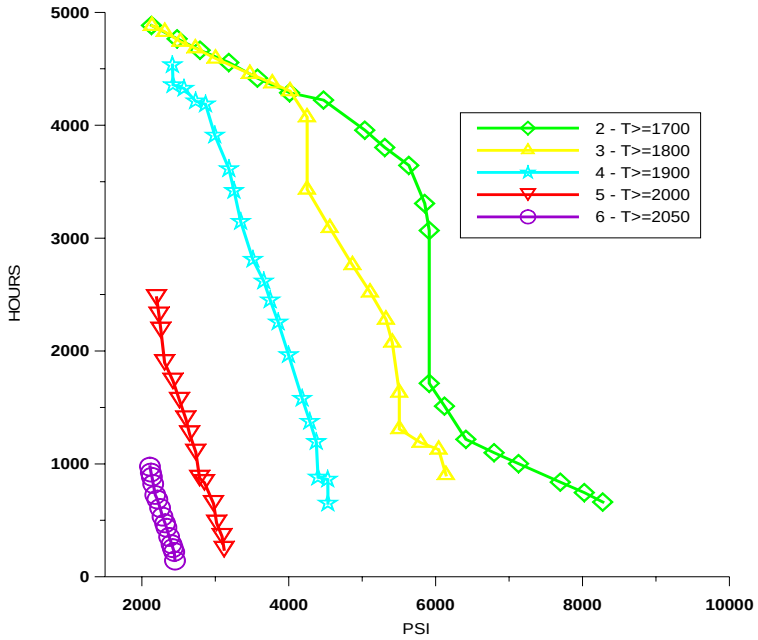


Fig. 15. Pareto-optimal sets for five different (temperature) constraints using 9 design variables.

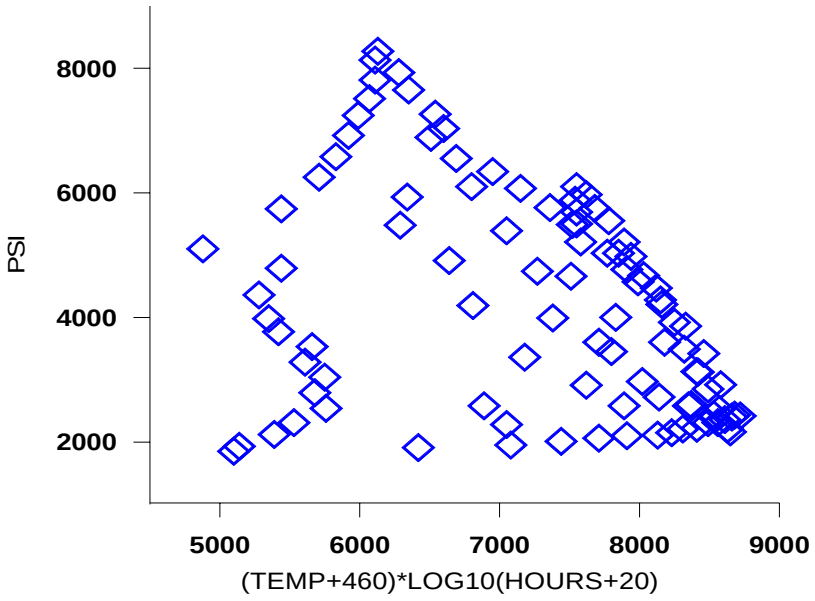


Fig. 16. Larsen-Mueller diagrams for two-criteria optimization problems using 9 design variables.

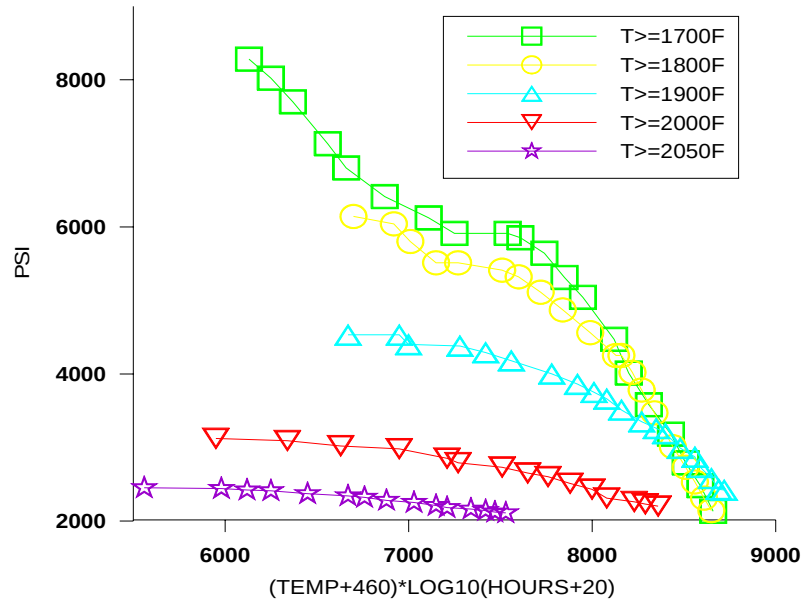


Fig. 17. Larsen-Mueller diagrams for five two-criteria optimization problems results using 9 design variables.

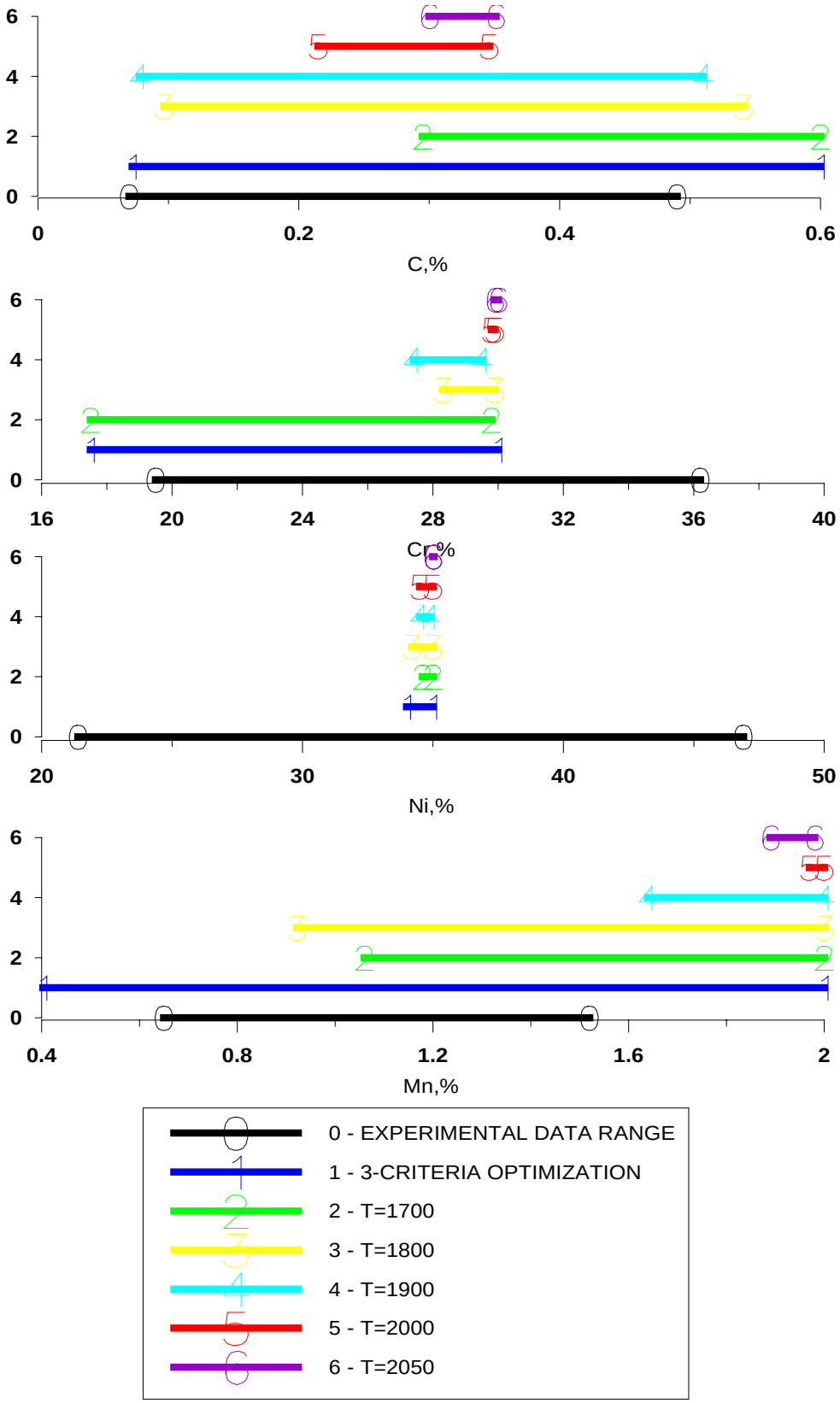


Fig. 18. Boundaries of variable parameters for sets of Pareto optimal solutions with 9 design variables.

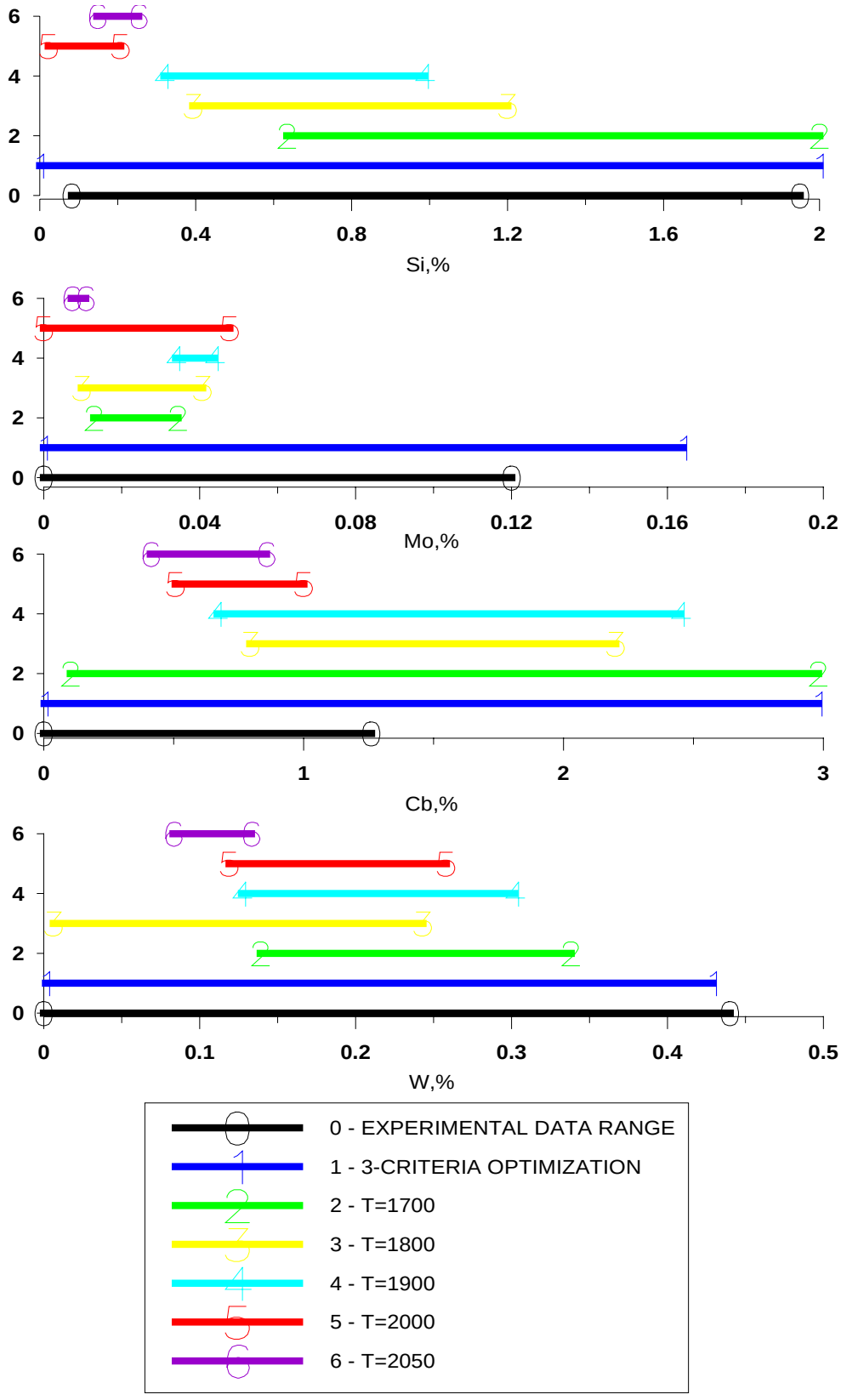


Fig. 19. Boundaries of variable parameters for sets of Pareto optimal solutions with 9 design variables.

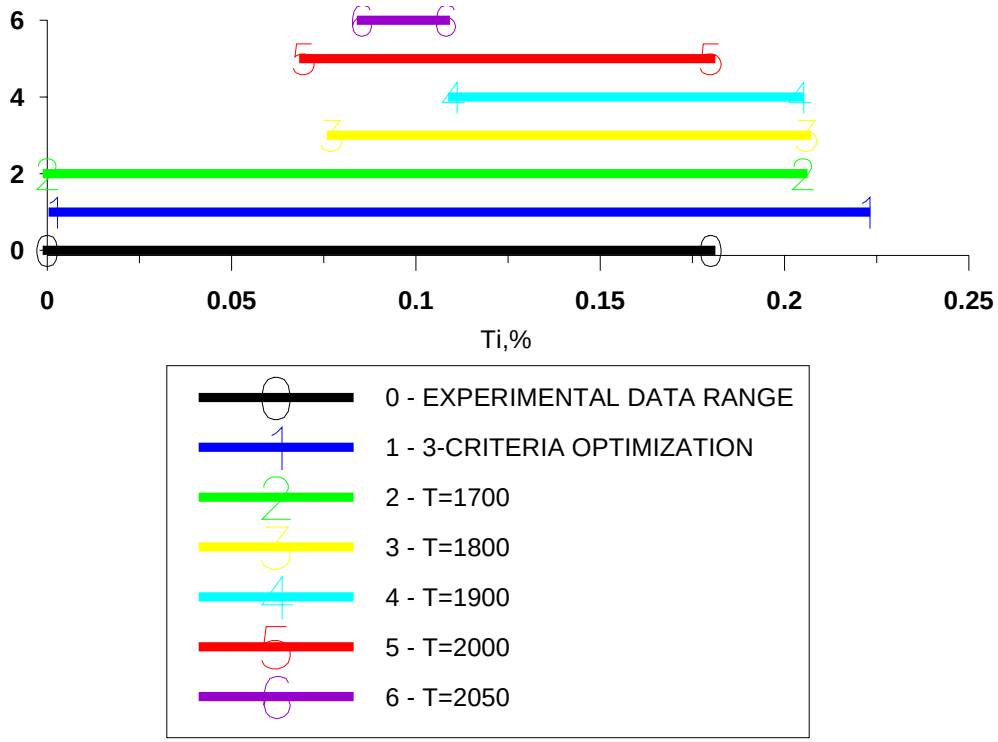


Fig. 20. Boundaries of variable parameters for sets of Pareto optimal solutions with 9 design variables.

5.4 Optimization Results for the Cases With 8 Design Variables

We then repeated this optimization run (three objectives) in which we used only 9 chemical elements as independent variables: ***C, Cr, Ni, Mn, Si, Mo, Cb, W***. Thus, *Titanium* was deleted from the previous case with 9 variables. We have followed the same steps during the optimization as when solving the problem with 17 variables. But, in this case there are differences. The variables' ranges were changed.

Table 3. Ranges of variation of 8 independent variables (chemical elements in the steel alloy)

	C	Cr	Ni	Mn	Si	Mo	Cb	W
min	0.00	17.50	25.00	0.00	0.00	0.00	0.00	0.00
max	0.60	30.00	35.00	2.00	2.00	2.00	3.00	2.00

The main reason of accuracy deterioration of the response surface representation is that while decreasing the number of variables for the same experimental data set, we added the additional noise.

5.4.1 Three-criteria optimization

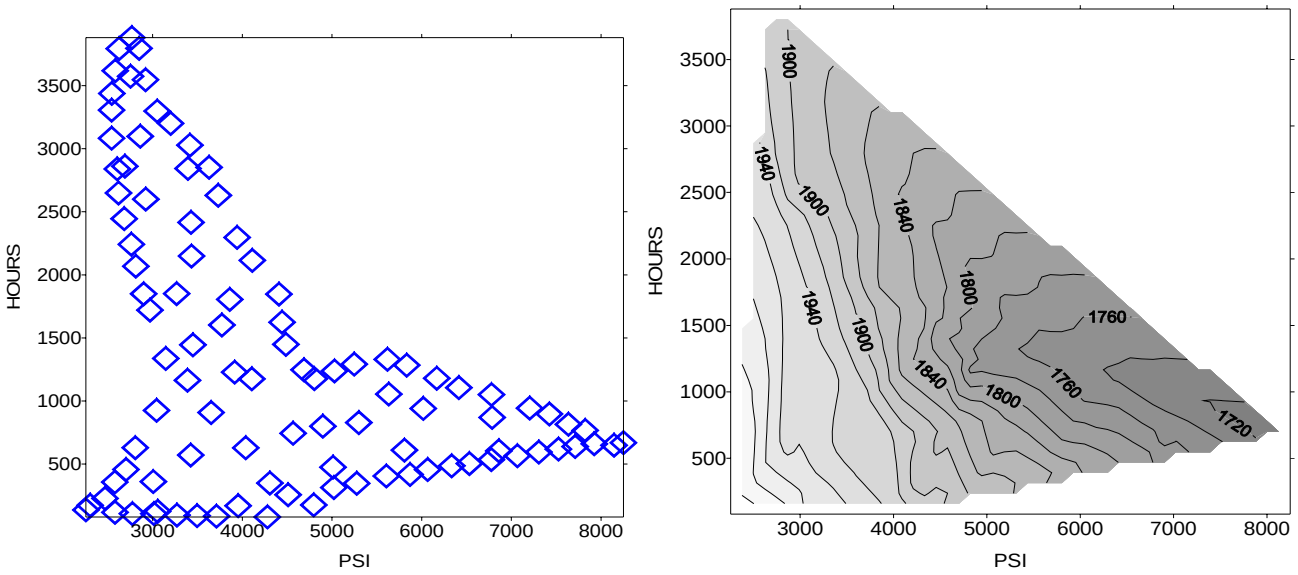


Fig. 21. Distribution of points in the objectives space using 8 design variables (chemical species).

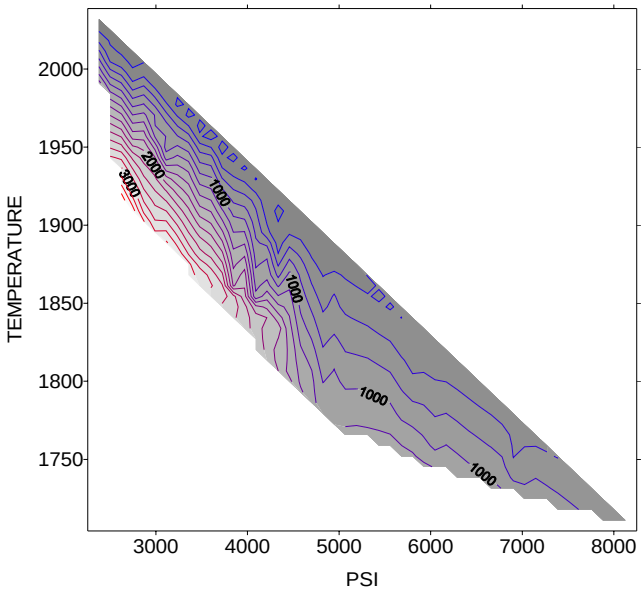


Fig. 22. Interdependence of optimization objectives for Pareto set using 8 design variables (chemical species).

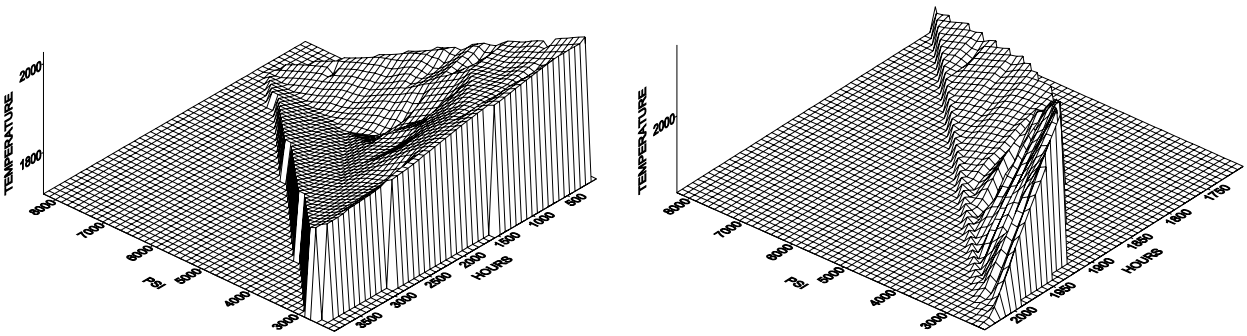


Fig. 23. Three-dimensional views of Pareto surfaces using 8 design variables (chemical species).

5.4.2 Two-objectives optimization (tasks N2,…,N5) using 8 design variables (chemical species)

Analysis of the three-criteria optimization results shows that there are no solutions with temperature less or equal 1600F. Because of this, we changed the value of constraint for the task N2. Constraint $T \geq 1600$ was replaced with $T \geq 1700$. Moreover, the constraint with $T \geq 2050$ has no feasible solutions in these test cases.

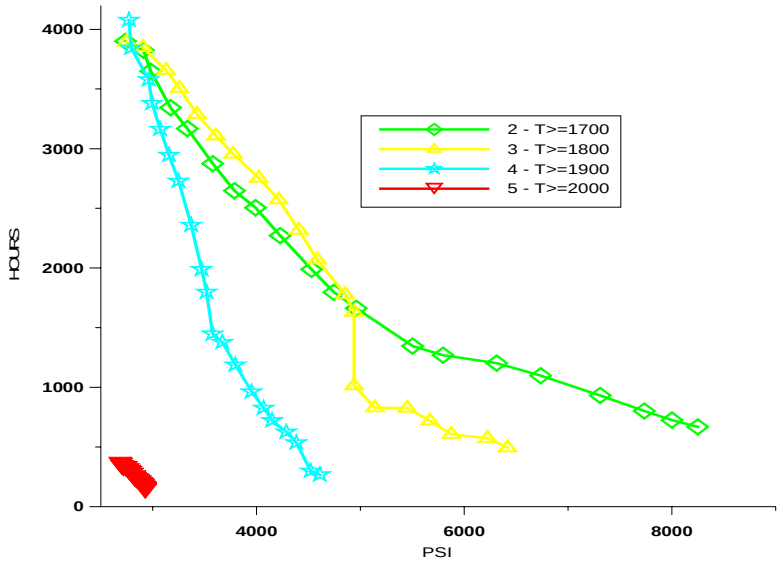


Fig. 24. Pareto-optimal sets using 8 design variables (chemical species).

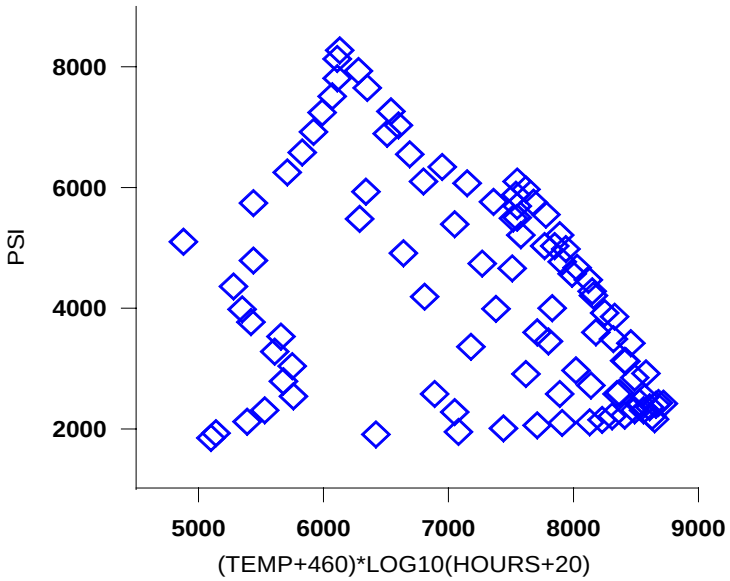


Fig. 25. Larsen-Mueller diagrams for three-criteria optimization: results using 8 design variables (chemical species).

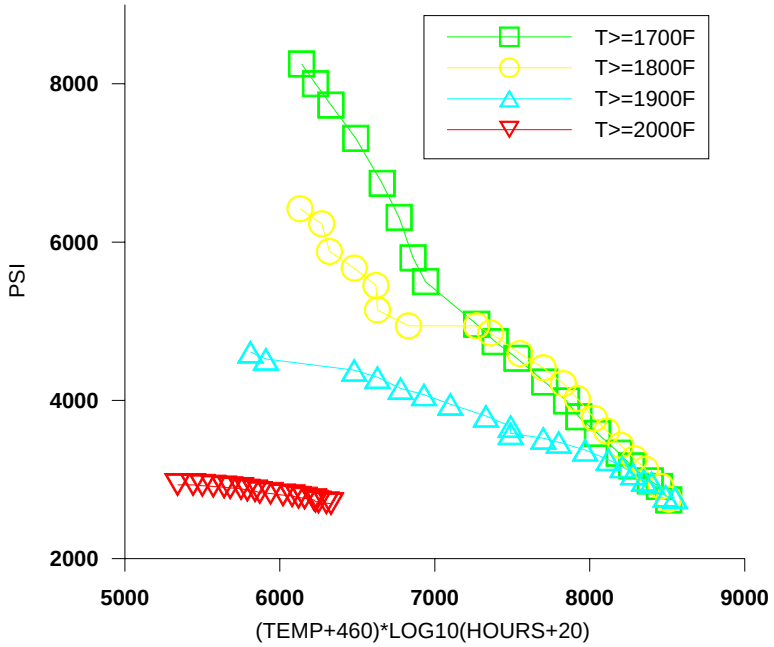


Fig. 26. Larsen-Mueller diagrams for two-criteria optimization: results using 8 design variables (chemical species).

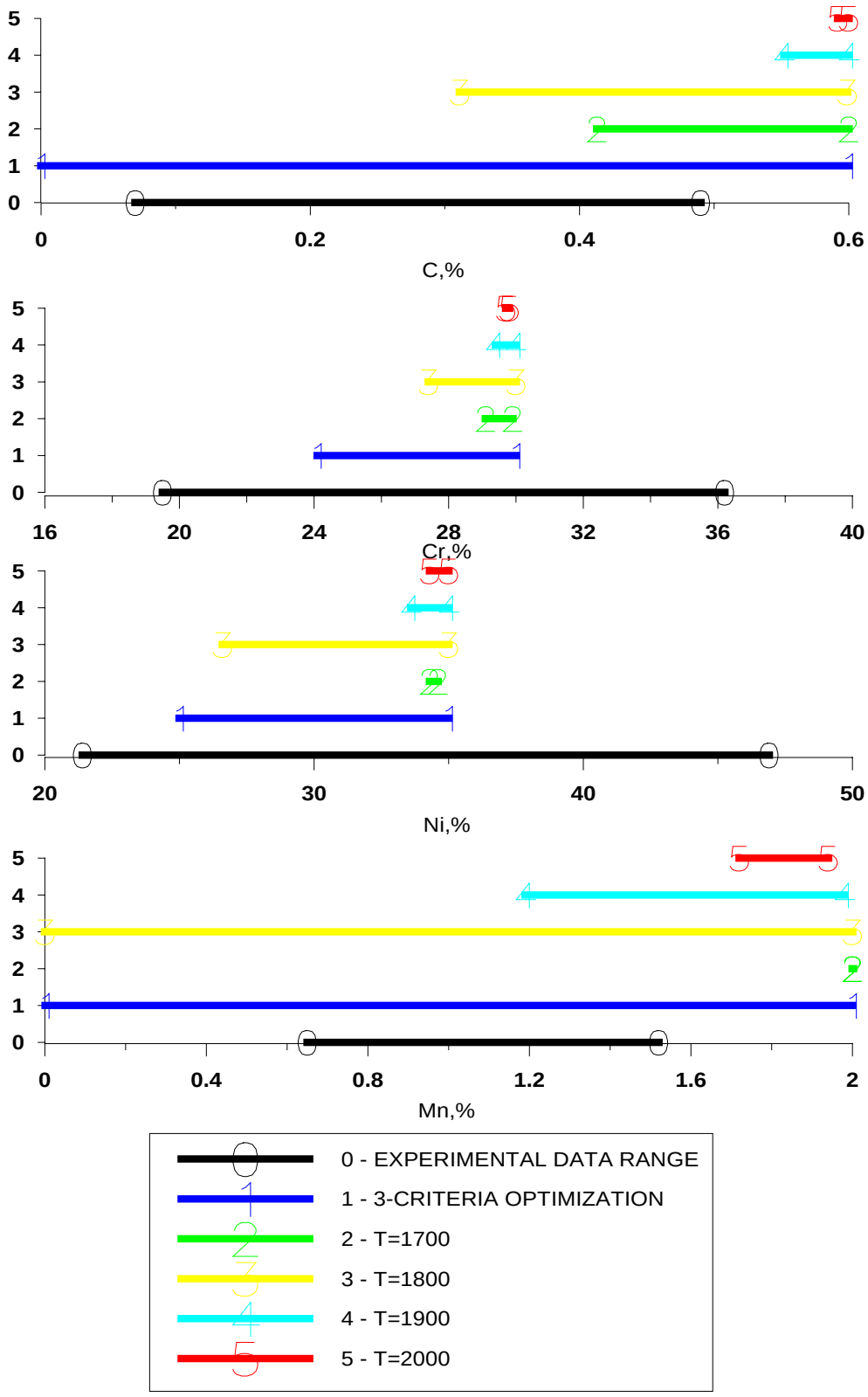


Fig. 27. Input data set and optimized ranges of chemical species using 8 design variables (chemical species).

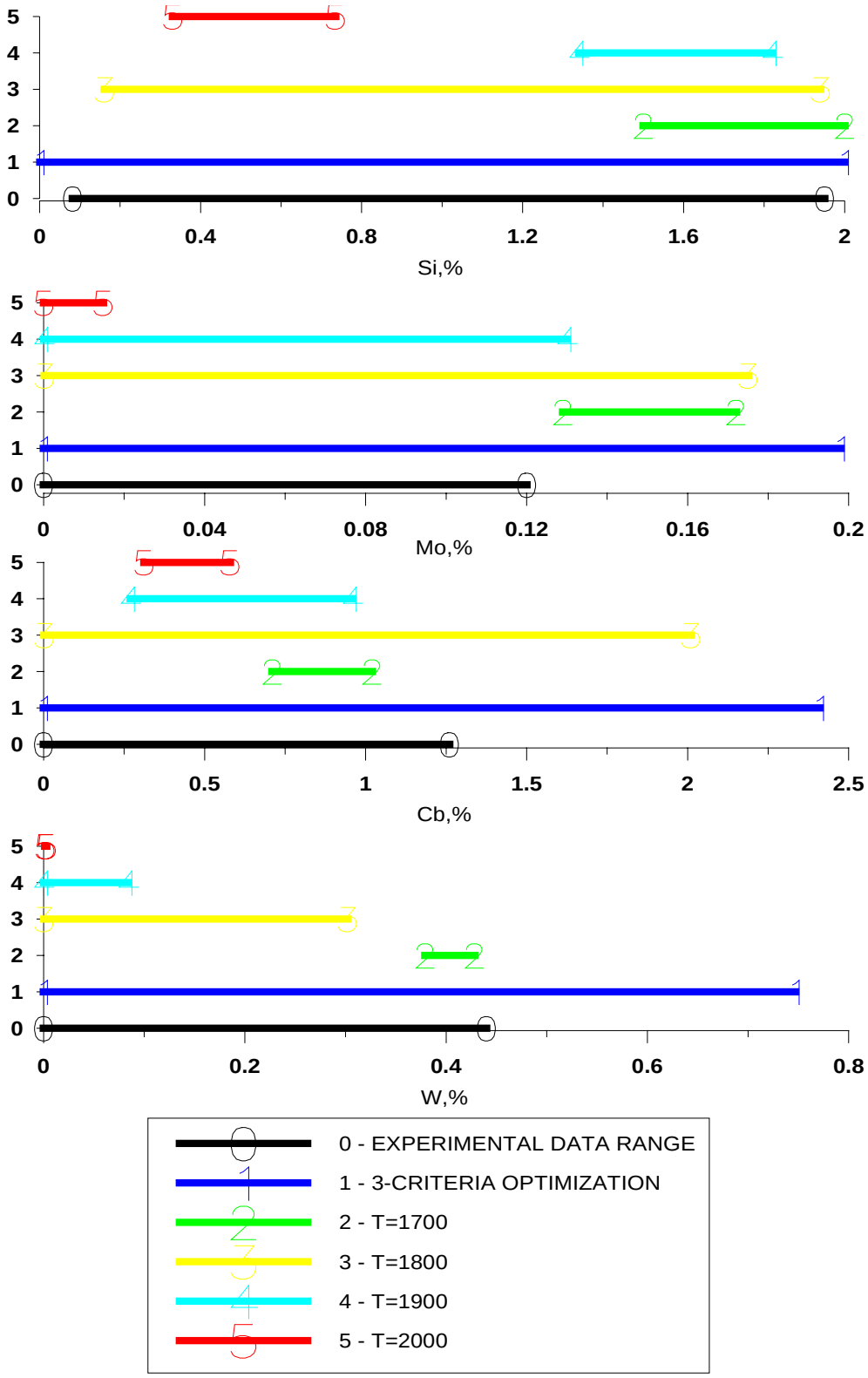


Fig. 28. Input data set and optimized ranges of chemical species using 8 design variables (chemical species).

5.5 Experimental Proof-of-the-Concept

We were unexpectedly faced with a situation where we could not use old experimental data base which we had before because a company that has been manufacturing our alloys and performing experimental evaluations of the thermo-mechanical properties of these alloys has abruptly changed their technology of producing such materials. That is, the old experimental data that was originally purchased corresponded to a different technological process. In addition, these experimental data had very bad distribution, which is why the approximation function (response surface analytical representation) had low level of accuracy.

This is the reason for a recent delay in our research and why we needed to obtain a new experimental data set. First, we created a new experimental plan. It had 120 ally compositions generated using Sobol's algorithm (Sobol, 1976) so that they are as uniformly distributed in the function space as possible thus creating conditions for very accurate response surface fit. We contracted these 120 steel alloys to be manufactured each having a specific different concentration of each of the seven elements. The chemical elements deemed to be important were *Ni, C, Cr, Co, W, Mo, Al, Ti*, *B, Nb, Ce, Zr, Y,* while the elements given in Table 4 were treated as extraneous impurities.

Table 4. Average percent of the extraneous species

S	P	Fe	Mn	Si	Pb	Bi
0.0037	0.006	0.085	0.013	0.067	0.0005	0.0005

Chemical elements whose concentrations were optimized were Ni, C, Cr, Co, W, Mo, Al, Ti. Concentration of Nb in all sample alloys was kept constant at 1.1 %, while concentrations of B, Ce, Zr, Y were kept at 0.025%, 0.015%, 0.04%, and 0.01%, respectively. Concentration of nickel was treated as represented by the amount remaining until completing 100 %. The design variables were allowed to vary within the limits given in Table 5.

Table 5. Ranges of variation of 7 chemical elements to be optimized

	C	Cr	Co	W	Mo	Al	Ti
min	0.13	8.0	9.0	9.5	1.2	5.1	2.0
max	0.20	9.5	10.5	11.0	2.4	6.0	2.9

Two simultaneous objectives of the alloy concentration optimization process were: maximize stress and maximize time until rupture at a fixed temperature of 975 degrees Celsius.

The experimental evaluation of the stress and life until rupture at a fixed temperature were performed for each of these 120 alloys (Table 6).

Then, we solved the optimization problem based on this experimental data, and found 20 Pareto set points (Table 7, columns 4,...,10).

Next, we had these 20 optimized concentrations manufactured and manufactured and experimentally tested (Table 7, columns 2 and 3; also Fig. 29). Consequently, seven new points of Pareto optimal set were found after the first iteration (they are points 121-125, 127 and 134 in Table 7). That is, we found 7 new steel alloy compositions so that each of them allows improvements of both objectives (Fig. 30).

Then, we solved a new optimization problem with all 140 points (120 original alloys plus 20 new Pareto set alloys). We found 20 new points of the Pareto set and we sent this information for the subcontractor to manufacture these 20 alloys, test them using classical experimental techniques, and provide us with these measured properties. We expect these results by early December of 2003. This constitutes the second iteration.

Total number of experimental points that we could afford on this project from the funds expended so far is 200. This is due to our limit of funds which we have budgeted for experimental research during this period. This means that we can afford to make only 4 iterations where each iterative stage has 20 new experimental points.

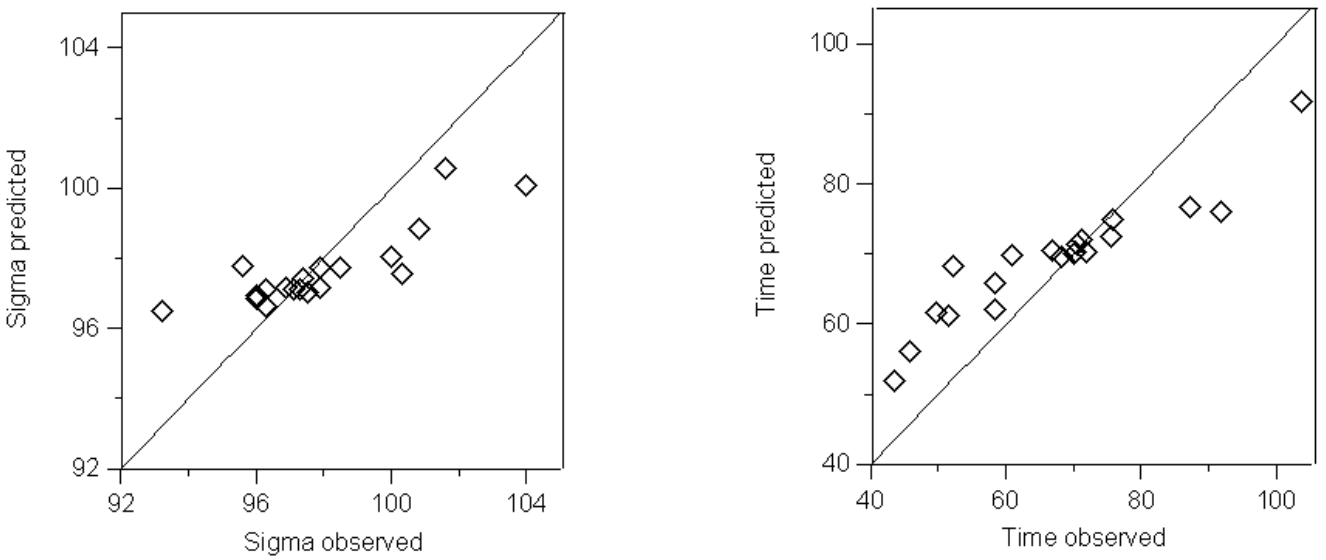


Fig. 29. Predicted and experimentally verified stress and life-time values after the first iteration.

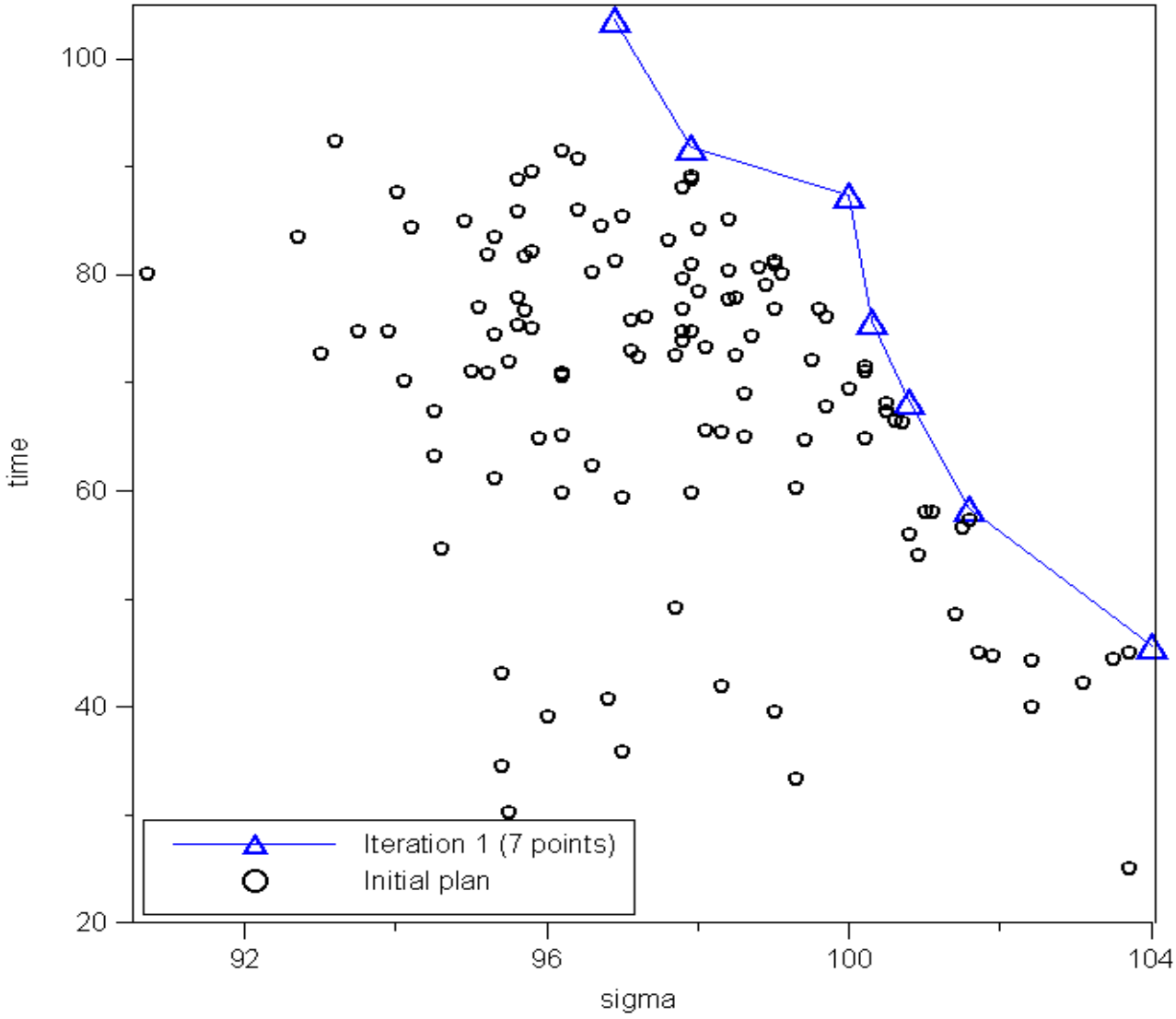


Fig. 30. The original experimental data set and the Pareto optimized new alloys after only one iteration.

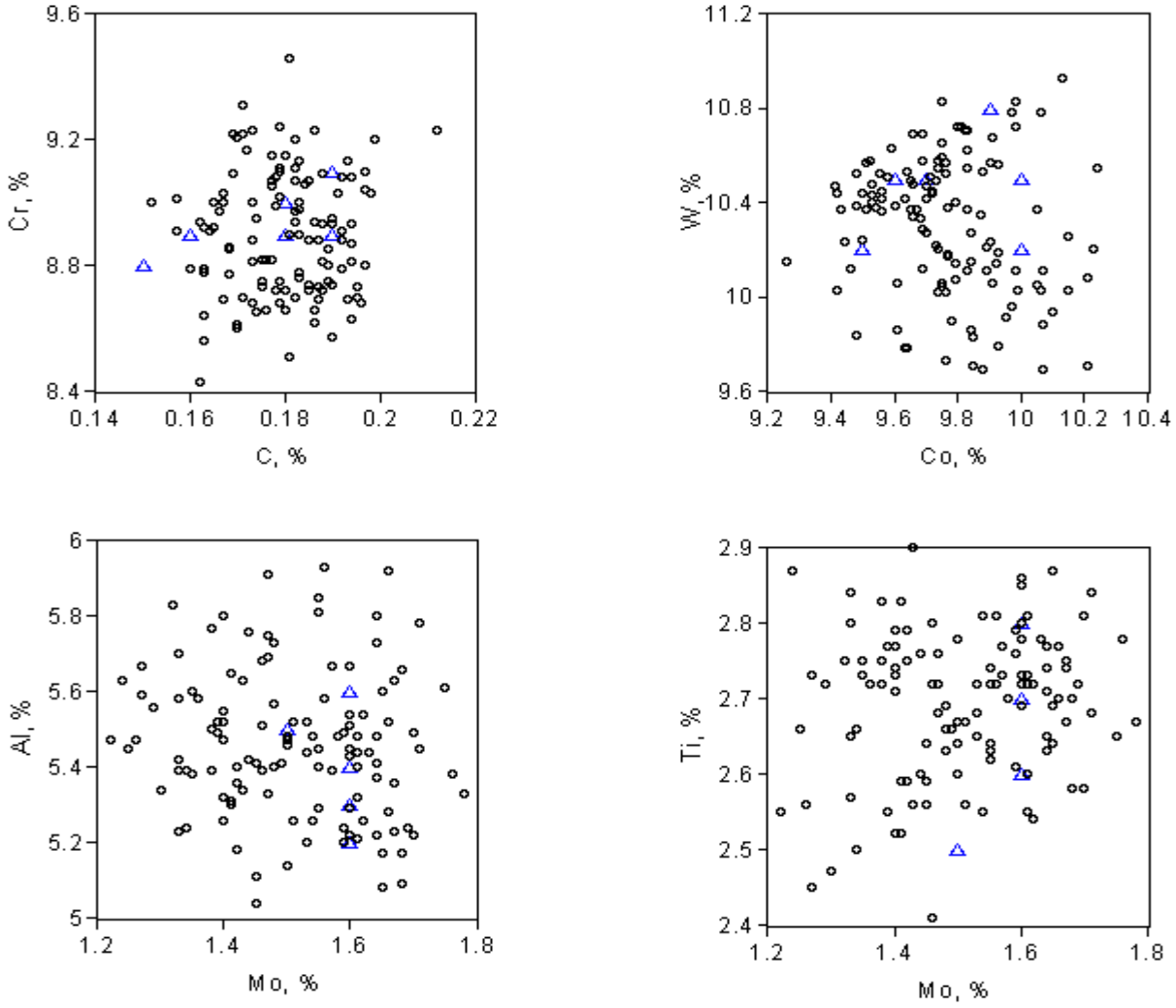


Fig. 31. Concentrations of different elements in the original data set and in the Pareto optimized set after the first iteration.

Table 6. Initial experimental data set for 120 steel alloys.

	Sigma, kg/mm^2	Time, hours	C, %	Cr, %	Co, %	W, %	Mo, %	Al, %	Ti, %
1	103.7	45.02	0.190	8.93	9.90	10.23	1.27	5.67	2.45
2	103.7	25.17	0.175	8.75	9.93	9.79	1.42	5.40	2.79
3	103.5	44.52	0.179	9.24	9.83	10.11	1.36	5.58	2.72
4	103.1	42.28	0.172	9.17	9.71	10.51	1.69	5.24	2.72
5	102.4	40.10	0.194	8.63	9.67	10.37	1.55	5.29	2.74
6	102.4	44.35	0.190	8.57	9.42	10.44	1.61	5.44	2.81
7	101.9	44.77	0.192	8.91	9.93	10.19	1.47	5.33	2.68
8	101.7	45.12	0.193	8.69	10.23	10.20	1.68	5.17	2.70
9	101.6	57.40	0.176	8.66	9.53	10.48	1.53	5.52	2.68
10	101.5	56.67	0.170	8.61	9.85	9.71	1.67	5.23	2.67
11	101.4	48.60	0.173	9.23	9.87	10.35	1.32	5.83	2.75
12	101.1	58.03	0.187	8.69	9.51	10.57	1.60	5.29	2.86

	Sigma, kg/mm^2	Time, hours	C, %	Cr, %	Co, %	W, %	Mo, %	Al, %	Ti, %
13	101.0	58.15	0.183	8.90	10.07	10.11	1.45	5.41	2.59
14	100.9	54.12	0.192	9.08	9.84	9.86	1.40	5.80	2.73
15	100.8	56.02	0.157	9.01	9.77	10.38	1.25	5.45	2.66
16	100.7	66.32	0.168	8.86	10.05	10.05	1.51	5.52	2.67
17	100.6	66.55	0.186	9.23	9.74	10.02	1.46	5.68	2.72
18	100.5	67.45	0.162	8.94	9.79	10.07	1.40	5.55	2.79
19	100.5	67.45	0.173	8.68	9.92	10.14	1.64	5.41	2.74
20	100.5	68.18	0.165	9.00	9.69	10.58	1.29	5.56	2.72
21	100.2	71.07	0.177	9.07	9.64	9.78	1.47	5.75	2.72
22	100.2	71.55	0.185	8.72	9.44	10.23	1.67	5.63	2.75
23	100.2	64.92	0.163	8.78	9.56	10.36	1.70	5.49	2.81
24	100.0	69.47	0.179	9.02	9.70	10.47	1.47	5.91	2.76
25	99.7	76.11	0.197	8.80	9.61	10.06	1.22	5.47	2.55
26	99.7	67.84	0.192	8.88	9.85	9.83	1.43	5.63	2.90
27	99.6	76.80	0.179	9.10	9.80	10.72	1.40	5.26	2.71
28	99.5	72.15	0.179	8.75	9.97	9.96	1.62	5.54	2.54
29	99.4	64.74	0.185	9.07	10.10	9.94	1.41	5.65	2.83
30	99.3	60.30	0.163	8.92	9.99	10.03	1.50	5.48	2.78
31	99.3	33.40	0.171	9.22	9.97	10.78	1.64	5.80	2.77
32	99.1	80.13	0.186	8.94	9.90	10.57	1.33	5.42	2.57
33	99.0	76.86	0.181	8.51	9.69	10.12	1.50	5.46	2.64
34	99.0	81.25	0.173	8.81	9.98	10.11	1.62	5.26	2.72
35	99.0	39.62	0.181	9.46	9.76	10.57	1.40	5.47	2.74
36	99.0	81.05	0.167	8.69	9.50	10.24	1.60	5.54	2.72
37	98.9	79.14	0.178	8.99	9.66	10.48	1.64	5.37	2.71
38	98.8	80.70	0.194	8.93	9.63	9.78	1.70	5.22	2.58
39	98.7	74.42	0.187	8.88	9.65	10.37	1.59	5.49	2.76
40	98.6	64.99	0.182	8.94	10.07	9.69	1.47	5.69	2.76
41	98.6	69.03	0.188	8.93	9.53	10.43	1.66	5.52	2.77
42	98.5	72.63	0.186	8.62	9.75	10.59	1.65	5.17	2.69
43	98.5	77.92	0.195	8.73	9.65	10.49	1.59	5.24	2.61
44	98.4	85.20	0.177	8.82	9.66	10.34	1.27	5.59	2.73
45	98.4	80.47	0.190	8.95	9.82	10.71	1.60	5.51	2.69

	Sigma, kg/mm^2	Time, hours	C, %	Cr, %	Co, %	W, %	Mo, %	Al, %	Ti, %
46	98.4	77.82	0.195	8.70	9.42	10.03	1.59	5.20	2.79
47	98.3	41.90	0.162	8.43	9.83	10.71	1.51	5.26	2.56
48	98.3	65.50	0.164	8.91	9.66	10.69	1.54	5.48	2.55
49	98.1	73.34	0.199	9.20	10.21	9.71	1.35	5.60	2.75
50	98.1	65.60	0.160	8.79	9.72	10.45	1.48	5.57	2.66
51	98.0	84.30	0.171	8.70	10.21	10.08	1.49	5.41	2.66
52	98.0	78.51	0.169	9.09	9.75	10.04	1.39	5.52	2.77
53	97.9	88.80	0.183	8.76	9.84	10.15	1.42	5.36	2.59
54	97.9	89.12	0.180	8.66	10.06	10.03	1.60	5.43	2.73
55	97.9	59.84	0.188	9.09	9.74	10.55	1.76	5.38	2.78
56	97.9	80.98	0.171	8.70	9.46	10.12	1.55	5.85	2.64
57	97.9	74.75	0.179	9.11	9.73	10.22	1.66	5.28	2.77
58	97.8	73.87	0.190	8.74	9.74	10.20	1.50	5.14	2.60
59	97.8	88.07	0.165	8.92	9.69	10.69	1.34	5.39	2.50
60	97.8	74.75	0.189	8.85	9.88	10.53	1.48	5.73	2.63
61	97.8	79.66	0.188	8.72	9.60	10.39	1.53	5.20	2.72
62	97.8	76.83	0.196	8.68	9.48	10.52	1.65	5.08	2.64
63	97.7	72.56	0.194	8.87	9.52	10.58	1.75	5.61	2.65
64	97.7	49.20	0.170	9.21	9.75	10.83	1.55	5.81	2.63
65	97.6	83.29	0.167	9.00	9.83	10.37	1.48	5.40	2.69
66	97.3	76.14	0.185	8.74	9.54	10.38	1.71	5.78	2.68
67	97.2	72.47	0.187	8.73	10.15	10.26	1.56	5.58	2.81
68	97.1	72.96	0.191	9.03	9.64	10.53	1.60	5.22	2.80
69	97.1	75.84	0.194	8.81	9.72	10.44	1.63	5.44	2.78
70	97.0	59.42	0.176	8.82	10.15	10.03	1.34	5.24	2.66
71	97.0	35.87	0.171	9.31	10.13	10.93	1.39	5.49	2.55
72	97.0	85.47	0.170	8.60	9.48	9.84	1.46	5.39	2.41
73	96.9	81.25	0.180	8.72	9.74	10.58	1.67	5.36	2.74
74	96.8	40.80	0.197	9.10	9.98	10.72	1.68	5.09	2.70
75	96.7	84.50	0.167	9.03	10.05	10.37	1.33	5.23	2.57
76	96.6	80.28	0.166	8.97	9.76	10.02	1.33	5.70	2.80
77	96.6	62.33	0.180	9.15	9.50	10.44	1.71	5.45	2.84
78	96.4	86.09	0.163	8.56	9.89	10.11	1.33	5.39	2.65

	Sigma, kg/mm^2	Time, hours	C, %	Cr, %	Co, %	W, %	Mo, %	Al, %	Ti, %
79	96.4	90.75	0.183	8.78	9.59	10.63	1.60	5.45	2.78
80	96.2	91.55	0.183	9.13	9.68	10.33	1.44	5.42	2.60
81	96.2	59.84	0.182	9.11	9.91	10.06	1.44	5.76	2.76
82	96.2	70.78	0.169	9.22	9.56	10.42	1.35	5.38	2.73
83	96.2	70.71	0.194	9.08	9.70	10.27	1.61	5.32	2.55
84	96.2	70.99	0.177	9.05	9.76	10.52	1.61	5.40	2.73
85	96.2	65.20	0.181	8.90	9.81	10.72	1.68	5.66	2.58
86	96.0	39.22	0.212	9.23	9.91	10.68	1.64	5.22	2.65
87	95.9	64.91	0.186	8.66	9.43	10.37	1.54	5.26	2.81
88	95.8	82.13	0.174	8.65	9.76	9.73	1.40	5.32	2.52
89	95.8	89.53	0.163	8.79	9.79	10.40	1.43	5.34	2.56
90	95.8	75.10	0.197	9.04	9.83	10.62	1.57	5.39	2.77
91	95.7	81.71	0.163	8.64	9.83	10.55	1.45	5.11	2.56
92	95.7	76.69	0.179	9.24	9.78	9.90	1.38	5.39	2.75
93	95.6	88.91	0.189	8.75	9.79	10.14	1.30	5.34	2.47
94	95.6	85.94	0.185	8.88	9.93	10.56	1.41	5.30	2.52
95	95.6	77.96	0.175	8.73	9.58	10.51	1.57	5.67	2.73
96	95.6	75.40	0.192	8.79	9.51	10.37	1.55	5.40	2.62
97	95.5	72.05	0.182	9.07	9.48	10.39	1.78	5.33	2.67
98	95.5	30.30	0.179	8.68	9.63	10.42	1.60	5.67	2.85
99	95.4	43.19	0.175	8.82	9.56	10.45	1.65	5.60	2.87
100	95.4	34.50	0.152	9.00	10.06	10.78	1.64	5.73	2.63
101	95.3	83.56	0.182	9.20	9.75	10.06	1.45	5.04	2.64
102	95.3	74.43	0.188	8.81	9.41	10.47	1.61	5.48	2.60
103	95.3	61.25	0.168	8.85	9.26	10.15	1.55	5.45	2.72
104	95.2	81.88	0.177	9.15	9.70	10.42	1.26	5.47	2.56
105	95.2	70.91	0.189	8.80	9.53	10.40	1.56	5.93	2.72
106	95.1	77.05	0.182	8.70	9.77	10.18	1.38	5.50	2.72
107	95.0	71.07	0.183	8.98	9.73	10.49	1.64	5.48	2.63
108	94.9	85.00	0.178	8.72	9.84	10.27	1.50	5.47	2.67
109	94.6	54.65	0.183	9.00	10.24	10.55	1.53	5.44	2.65
110	94.5	67.43	0.193	9.13	9.75	10.65	1.61	5.21	2.72
111	94.5	63.30	0.169	9.22	9.69	10.29	1.40	5.52	2.77

	Sigma, kg/mm^2	Time, hours	C, %	Cr, %	Co, %	W, %	Mo, %	Al, %	Ti, %
112	94.2	84.46	0.173	8.88	9.98	10.83	1.41	5.31	2.59
113	94.1	70.17	0.184	9.06	9.44	10.23	1.66	5.92	2.70
114	94.0	87.63	0.182	8.97	9.61	9.86	1.24	5.63	2.87
115	93.9	74.83	0.174	8.95	9.89	10.21	1.42	5.18	2.75
116	93.5	74.73	0.198	9.03	9.88	9.69	1.33	5.58	2.84
117	93.2	92.38	0.168	8.77	9.95	9.91	1.58	5.48	2.70
118	93.0	72.70	0.157	8.91	9.77	10.17	1.46	5.51	2.80
119	92.7	83.60	0.178	9.08	9.55	10.52	1.65	5.60	2.69
120	90.7	80.10	0.173	9.00	10.07	9.88	1.38	5.77	2.83

Table 7. Experimental verification of 20 optimized alloy compositions after the first iteration.

	Sigma, kg/mm^2	Time, hours	C, %	Cr, %	Co, %	W, %	Mo, %	Al, %	Ti, %
121	104.0	45.7	0.196	9.13	9.94	10.52	1.56	5.28	2.62
122	101.6	58.3	0.162	8.88	9.94	10.16	1.60	5.60	2.63
123	100.8	68.3	0.182	8.90	9.95	10.86	1.55	5.34	2.84
124	100.3	75.7	0.188	8.92	9.64	10.57	1.60	5.67	2.77
125	100.0	87.3	0.187	9.00	9.51	10.26	1.52	5.47	2.65
126	98.5	70.3	0.172	8.98	9.85	10.63	1.63	5.23	2.70
127	97.9	91.8	0.179	8.95	9.69	10.54	1.60	5.14	2.67
128	97.9	70.4	0.181	9.21	9.79	10.52	1.60	5.46	2.74
129	97.9	66.8	0.182	8.84	9.49	10.57	1.60	5.75	2.69
130	97.5	51.5	0.190	9.04	9.54	10.30	1.70	5.74	2.80
131	97.4	70.1	0.143	8.74	9.73	10.45	1.55	5.21	2.56
132	97.3	49.6	0.182	8.90	9.87	10.78	1.68	5.40	2.62
133	97.1	60.8	0.183	8.93	9.68	10.53	1.64	5.32	2.60
134	96.9	103.7	0.144	8.85	9.66	10.43	1.50	5.52	2.42
135	96.3	43.5	0.193	9.30	9.87	10.78	1.68	5.47	2.73
136	96.3	52.2	0.185	8.88	9.53	10.36	1.61	5.30	2.62
137	96.0	75.5	0.198	9.03	9.68	10.49	1.53	5.28	2.74
138	96.0	58.3	0.186	8.92	9.75	10.73	1.74	5.44	2.86
139	95.6	71.2	0.199	8.70	9.71	10.51	1.65	5.10	2.65
140	93.2	71.8	0.191	8.51	9.53	10.33	1.59	5.49	2.55

5.6 The Concept of Inverse Design of Alloy Compositions

Our research during the last quarter concentrated on the inverse method in predicting chemical composition of steel alloys. It is a highly innovative approach that has received a warm welcome by some of the materials engineering experts from industry. For example, this formulation allows a structural design engineer who designed a machine part to ask a materials scientist to provide him with a precise chemical composition of an alloy that will sustain a specified stress level, at a specified temperature, and last for a specified number of hours. This inverse method uses a variant of Prof. Yegorov's stochastic optimizer to determine not one, but a number of alloys (Pareto front points) each of which will satisfy the desired specifications while having different percentages of each of the alloying elements. This provides the customer with increased flexibility when deciding to create such an alloy because he/she can use the "recipe" which is made of the most readily available and the cheapest elements on the market at that point in time.

Several mathematical formulations and corresponding software packages have been developed for different ways how to achieve inverse determination of chemical compositions of alloys satisfying a set of specified mechanical and cost/availability properties. These different formulations were then compared and analytically evaluated in an attempt to determine the most appropriate formulation. This way, the customer can choose the optimized alloy composition that is the most available and the least expensive at a moment when it is ordered from the alloy manufacturer.

The basic version of the licensed semi-stochastic multi-objective optimization software called IOSO was augmented so that now it can handle up to 14 simultaneous design objectives. When testing samples of actual alloys, there is always certain level of measurement error due to the finite accuracy of the testing equipment. This level of expected accuracy can now be specified and the results of the alloy composition optimization will automatically be modified to reflect this degree of uncertainty. Furthermore, during the manufacturing (melting and casting/solidification) of each new alloy, there is always a degree of uncertainty if the resulting alloy will have precisely the chemical composition that was expected when preparing and measuring the alloying components' masses. The level of this uncertainty depends on the level of sophistication of the alloy producing process. Now, we have incorporated this feature in our alloy optimization software, whereby the materials designer can specify the accuracy level of the manufacturing process and the optimizer will automatically and appropriately modify the predicted quantities.

In this problem the percentages of the following 14 elements were treated as independent variables:

C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti.

The ranges of these elements were set as follows. First, minimum and maximum values for existing set of experimental data ($Expmin_i$, $Expmax_i$ = i = 1,..,14) were defined. Then, new minimum and maximum values for each of the 14 elements were obtained according to the following simple dependencies: ($Min_i = 0.9\ Expmin_i$, $Max_i = 1.1\ Expmax_i$ = i = 1,….,14). These ranges are given in Table 8.

Table 8. Ranges of variation of 14 independent variables during inverse alloy design optimization

	C	S	P	Cr	Ni	Mn	Si
min	0.063	0.001	0.009	17.500	19.300	0.585	0.074
max	0.539	0.014	0.031	39.800	51.600	1.670	2.150

	Mo	Co	Cb	W	Sn	Zn	Ti
min	0.000	0.000	0.000	0.000	0.000	0.001	0.000
max	0.132	0.319	1.390	0.484	0.007	0.015	0.198

The inverse problem in design of alloys is determination of chemical composition(s) of alloy(s) that will provide specified levels of, for example, stress at a specified temperature for the specified length of time. The inverse problem can be then formulated as, for example, a multi-objective optimization problem with a given set of equality constraints. We have used IOSO stochastic optimization algorithm to achieve the solution of this type of inverse alloy design problem. The results are shown in a sequence of figures presented on pages 9-16. It should be pointed out that these are the visualizations of only two (Cr and Ni) of the 14 chemical elements listed above and optimized in order to illustrate how the method works.

When the temperature and the life expectancy are unconstrained (unspecified) the optimizer will give a fairly large domain for possible variations of the concentrations of Cr and Ni. But, as the constraints on temperature level are introduced and progressively increased, the feasible domain for varying Cr and Ni will start to shrink. Similar general trend can be observed when the life expectancy is specified and progressively increased. Finally, when temperature level and the life expectancy are prescribed simultaneously and progressively increased simultaneously, the feasible domain for concentrations of Cr and Ni rapidly reduces. Numbered iso-contours in all of these figures represent the stress level. Similar patterns could be obtained when looking at any other pair of alloying elements.

Inverse problem of determining chemical compositions of alloys

(formulation # 1)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (multi- objective statement – 3 simultaneous objectives)

- Stress (PSI) ***(PSI-PSI req.)**2 –> minimize***
- Operating temperature (T) ***(T-T req.)**2 –> minimize***
- Time to "survive" until rupture (Hours) ***(Hours-Hours req.)**2 –> minimize***

constraints: have none

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 2)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (single-objective statement)

- Stress (PSI);
- Operating temperature (T);
- Time to "survive" until rupture (Hours).

(PSI-PSI req.)**2+ (T-T req.)**2+ (Hours-Hours req.)**2 –> minimize

constraints: have none

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 3)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (multiple-objectives statement – 3 simultaneous objectives)

- Stress (PSI);
- Operating temperature (T);
- Time to "survive" until rupture (Hours).

constraints: ***(PSI-PSI req.) –> minimize;***
(T-T req.) –> minimize;
(Hours-Hours req.) –> minimize

constraints: have none

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 4)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (single-objective statement)

- Stress (PSI);
- Operating temperature (T);
- Time to "survive" until rupture (Hours).

(PSI-PSI req.)**2+ (T-T req.)**2+ (Hours-Hours req.)**2 –>minimize

constraints: ***PSI-PSI req.) –> minimize;***
(T-T req.) –> minimize;
(Hours-Hours req.) –> minimize

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 5)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (single-objective statement)

- Stress (PSI);
- Operating temperature (T);
- Time to "survive" until rupture (Hours).

(PSI-PSI req.)**2–>minimize

constraints: ***(T-T req.) –> minimize;***
(Hours-Hours req.) –> minimize

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 6)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (single-objective statement)

- Stress (PSI);
- Operating temperature (T);
- Time to "survive" until rupture (Hours).

(T-T req.)**2 –> minimize

constraints: ***PSI-PSI req.) –> minimize;***
(Hours-Hours req.) –> minimize

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 7)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (single-objective statement)

- Stress (PSI);
- Operating temperature (T);
- Time to "survive" until rupture (Hours).

(Hours-Hours req.)**2 –> minimize

constraints: ***PSI-PSI req.) –> minimize;***
(T-T req.) –> minimize;

mathematical model: have none; use an existing database

Inverse problem of determining chemical compositions of alloys

(formulation # 8)

Purpose: Determine chemical composition of an alloy that will have specified (desired) properties

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criteria: (multi- objective statement – 10 simultaneous objectives)

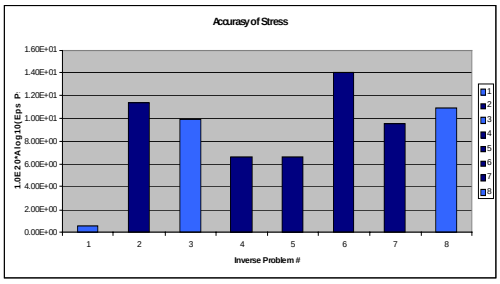
- Stress (PSI) ***(PSI-PSI req.)**2 –> minimize***
- Operating temperature (T) ***(T-T req.)**2 –> minimize***
- Time to "survive" until rupture (Hours) ***(Hours-Hours req.)**2 –> minimize***

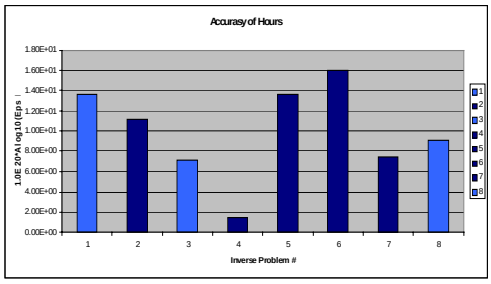
Cr -> minimize; Ni->minimize; Mo->minimize; Co->minimize; Cb >minimize; W >minimize; Sn >minimize; Zn >minimize; Ti >minimize;

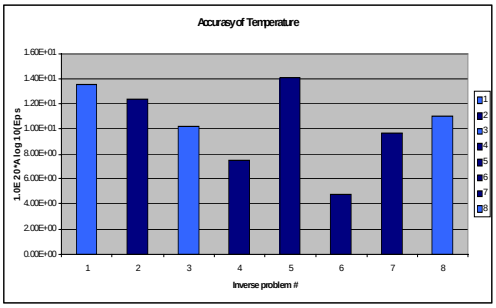
constraints: have none

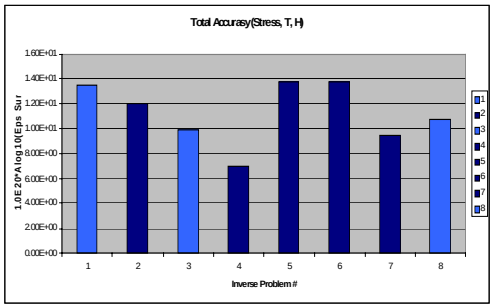
mathematical model: have none; use an existing database

Comparative analysis of accuracy of satisfying prescribed stress, temperature, life expectancy and their combination for inverse formulations # 1 to #8

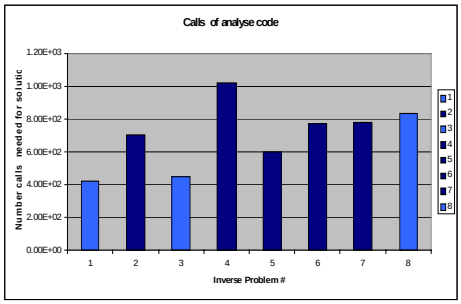


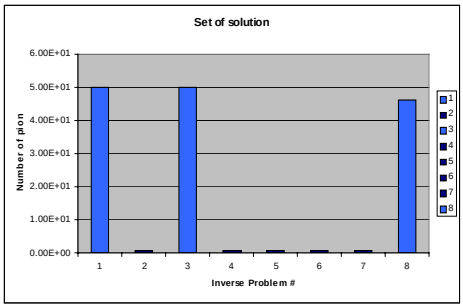


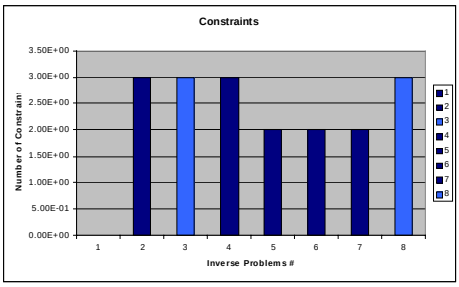


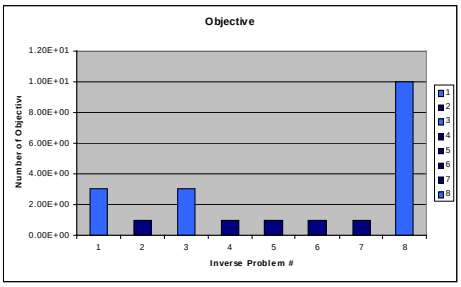


Comparison of various parameters (number of analysis needed, number of constraints, number of Pareto points, number of objectives) used in inverse formulations # 1 to #8)









Mathematical criteria for comparative analysis of different inverse formulations for determining chemical compositions of alloys

$$Score = K_1 * K_2 * (Eps) / K_3 \rightarrow Maximize$$

$$Eps = SUM\left(* 1/ \left((PSI-PSI\ req.)^{**}2 + (T-T\ req.)^{**}2 + (Hours-Hours\ req.)^{**}2 \right)\right)$$

$$K_1 = 10*N_{object} + N_{Constr} + N_{design}$$

$$K_2 = 100* Del_{PSI} + Del_{T} + Del_{Hours}$$

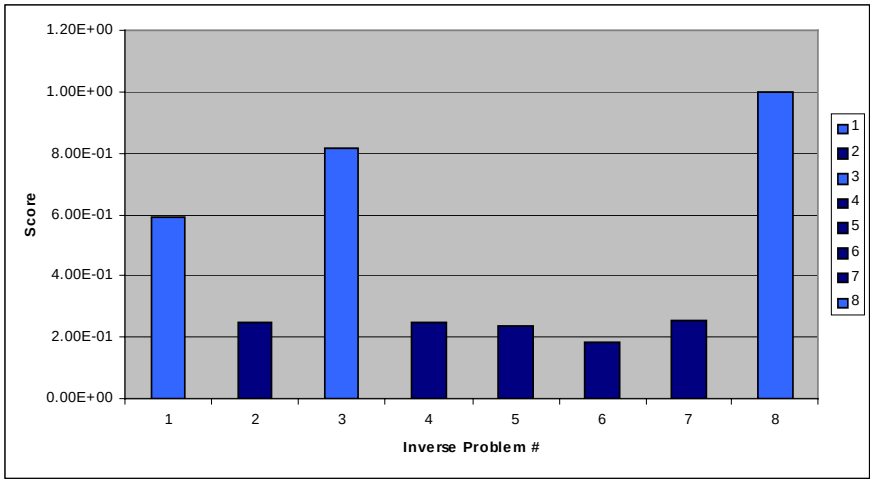
$$Del_{PSI} = 1- (PSI-PSI\ req.) / PSI\ req.$$

$$Del_{T} = 1- (T-T\ req.) / T\ req.$$

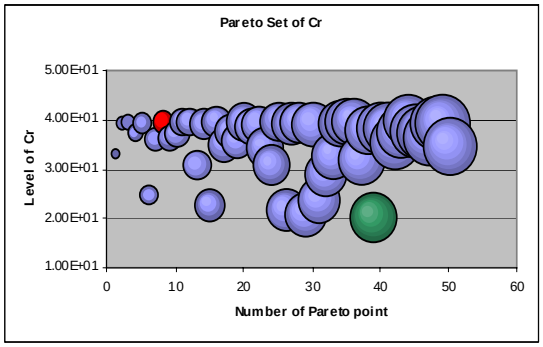
$$Del_{Hours} = 1- (Hours-Hours\ req.) / Hours\ req.$$

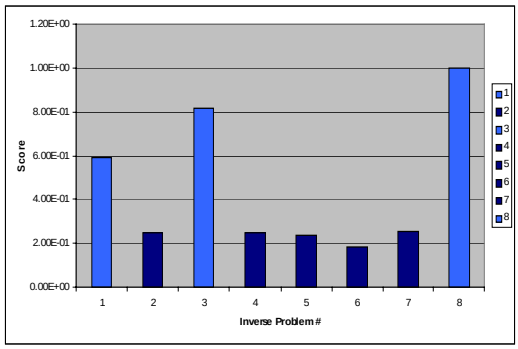
$$K_3 = N\ calls / N_{Poreto}$$

Comparative analysis of overall performance of different inverse formulations for determining chemical compositions of alloys (formulations # 1 to #8)



Comparative analysis of different inverse formulations for determination of chemical compositions of alloys

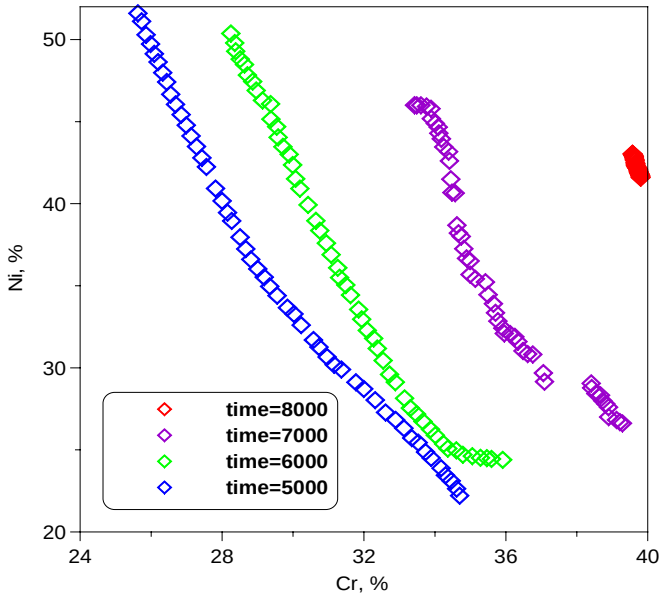




	Eps str	*Eps t*	*Eps h*	*Eps sum*	*N Const*	*N Obj*	*N Point (Poreto)*	*N Calls*	*Score*
Prob.1	.408E-19	.356E-06	.536E-06	.297E-06	0	3	50	417	0.590
Prob.2	.269E-08	.267E-07	.172E-08	.104E-07	3	1	1	703	0.246
Prob.3	.897E-10	.143E-09	.134E-12	.777E-10	3	3	50	445	0.817
Prob.4	.434E-13	.289E-12	.244E-18	.111E-12	3	1	1	1020	0.246
Prob.5	.413E-13	.139E-05	.549E-06	.646E-06	2	1	1	601	0.239
Prob.6	.954E-06	.576E-15	.980E-04	.646E-06	2	1	1	774	0.180
Prob.7	.408E-10	.515E-10	.299E-12	.309E-10	2	1	1	776	0.256
Prob.8	.714E-09	.928E-09	.127E-10	.552E-09	3	10	46	834	1.000

Multicriteria optimization of material composition for preset properties (inverse problem) using method #3

Number of variables (alloying elements): 14.
Criteria: determine Cr and Ni concentrations.



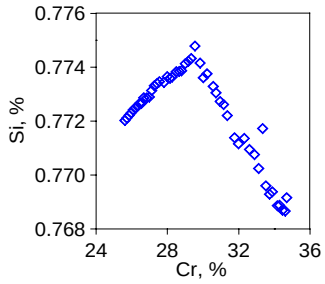
Constraints:
Stress=4000;
Temperature=1800;
Time=preset time.

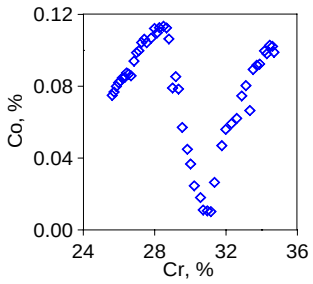
This approach allows us to vary the chemical composition for the same properties !

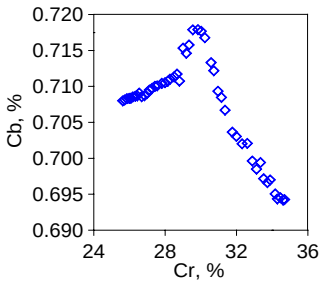
Multicriteria optimization of material composition for preset properties (inverse problem) using formulation #3

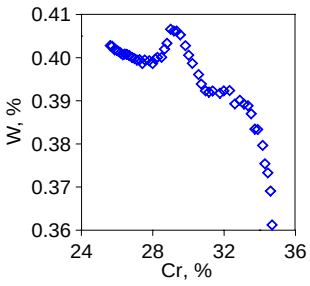
Number of variables (alloying elements): 14.
Criteria: determine Cr and Ni concentrations.

Constraints:
Stress=4000
Temperature=1800
Time=5000.









This approach allows us to vary the chemical composition for the same properties !

Optimization of chemical compositions of alloys

Purpose: Optimization of chemical composition of an alloy by a number of criteria with the use of an existing database

Problem features:

variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criterion: *for a given level of response surface accuracy for properties of alloy* :

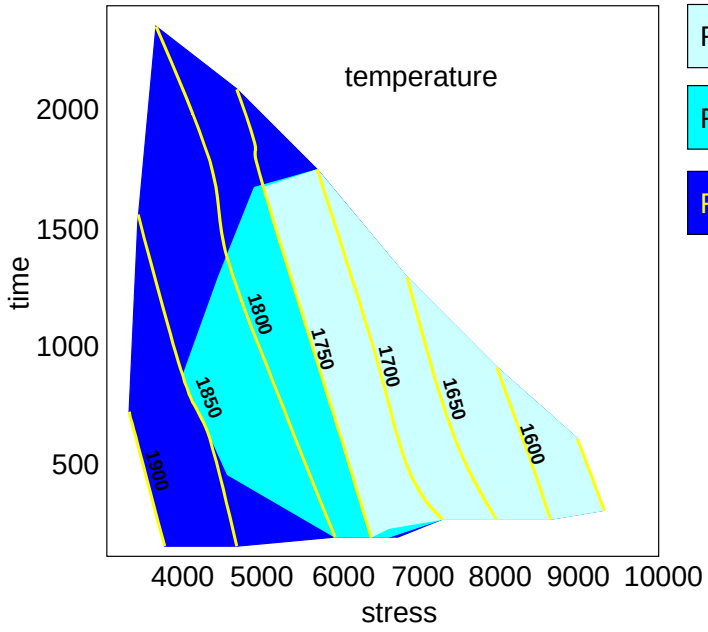
- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

response surface accuracy

mathematical model: have none; use an existing database

Multicriteria optimization of material properties taking into account the response surface accuracy

Criteria: stress, time, temperature.
Constraint: response surface accuracy.



Response surface error < 10%

Response surface error < 20%

Response surface error < 50%

This approach enables us to ensure higher levels of reliability of realization for optimized solutions !

Optimization of chemical compositions of alloys

Purpose: Optimization of chemical composition of an alloy by a number of criteria, with the use of existing database

Problem features:

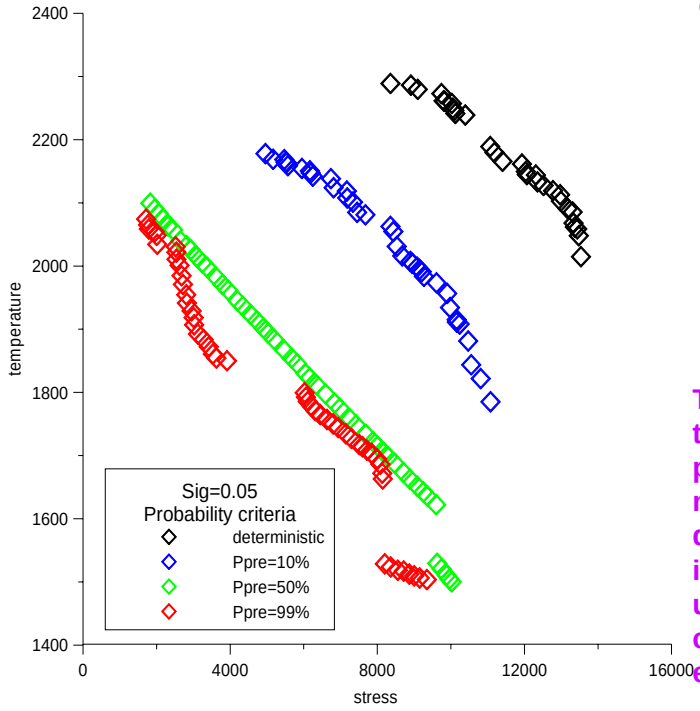
variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** (14 variables).

criterion: *for a given level of probability for properties of alloy* :

- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

mathematical model: have no, the use of existing database

Multicriteria optimization of material properties by probability criteria



Criteria: stress and temperature which are ensured with preset probability;

Constraint: time ensured with preset probability.

Condition: chemical elements concentrations are distributed by normal law with sigma=0.05

This approach enables us to achieve higher levels of probability of manufacturing the designed alloys by taking into account the uncertainty of the actual concentrations of alloying elements.

Optimization of chemical compositions of alloys

Purpose*:* Optimization of chemical composition of an alloy by a number of criteria, with the use of existing database

Problem features:

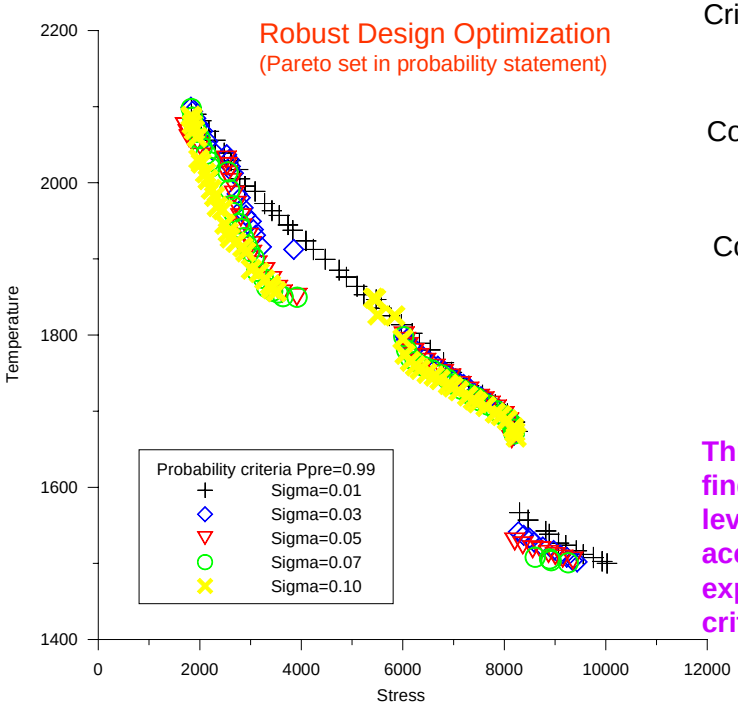
variable parameters: chemical composition of an alloy ***C, S, P, Cr, Ni, Mn, Si, Mo, Co, Cb, W, Sn, Zn, Ti*** for given level of accuracy (14 variables).

criterion: *for given level of probability for properties of alloy :*

- Stress (PSI – maximize);
- Operating temperature (T – maximize);
- Time to "survive" until rupture (Hours – maximize).

mathematical model: have none; use an existing database

Multicriteria optimization of material properties by probability criteria



Criteria: stress and temperature which are ensured with preset probability;

Constraint: time ensured with preset probability.

Condition: chemical elements concentrations are distributed by normal law with sigma=0.05

This approach allows us to find solutions with a <u>given</u> level of manufacturing accuracy with life time expectancy probability criteria of 50%.

6. Listing of All Publications and Technical Reports Supported Under This Grant or Contract

1. Semi-Stochastic Optimization of Chemical Composition of High-Temperature Austenitic Steels for Desired Mechanical Properties (Dulikravich, G. S., Yegorov, I. N., Sikka, V. N. and Muralidharan, G.), 2003 TMS Annual Meeting, Yazawa International Symposium: Processing and Technologies, TMS Publication, (eds: Kongoli, F., Itakagi, K., Yamaguchi, C. and Sohn, H.-Y.), Vol. 1, pp. 801-814, San Diego, CA, March 2-6, 2003.
2. Materials-by-Design: Direct and Inverse Problems Using Robust Stochastic Optimization (Dulikravich, G. S., Yegorov, I. N., Sikka, V. N. and Muralidharan, G.) accepted as an *Invited Lecture*, Symposium on "Materials by Design: Atoms To Applications", 2004 Annual Meeting of TMS, Charlotte, NC, March 14-18, 2004.
3. Superalloys Direct and Inverse Design Using Self-Adapting Response Surface Optimization (Dulikravich, G. S., Yegorov, I. N., Sikka, V. N. and Muralidharan, G.), International Symposium on Inverse Problems, Design and Optimization – IPDO, Rio de Janeiro, Brazil, March 17-19, 2004.
4. Inverse Design of Alloys for Specified Stress, Temperature and Time-to-Rupture by Using Stochastic Optimization (Yegorov, I. N. and Dulikravich, G. S.), 10th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Albany, NY, Aug. 30 – Sept. 1, 2004.

7. List of all participating scientific personnel showing any advanced degrees earned by them while employed on the project

There were no advanced degrees earned by students while working on this project.

8. Report of inventions (by title only)

There were no patents or inventions filed.

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10. Appendixes

Appendix 1

first.xls

PSI	DEGREE F	HOURS	C	S	P	Cr	Ni	Mn	Si	Cu	Mo	Pb	Co
3498.000	1850.000	1587.000	0.410	0.007	0.013	27.700	46.210	0.700	1.270	0.080	0.021	0.002	0.020
6998.000	2100.000	53.000	0.033	0.009	0.016	20.730	60.520	0.410	0.530	0.050	9.630	0.004	0.006
6998.000	1700.000	83.000	0.033	0.009	0.016	20.730	60.520	0.410	0.530	0.050	9.630	0.004	0.006
6998.000	1700.000	45.000	0.033	0.009	0.016	20.730	60.520	0.410	0.530	0.050	9.630	0.004	0.006
2802.000	2000.000	24.000	0.409	0.010	0.017	24.310	35.400	0.790	1.520	0.080	0.050	0.001	0.150
2817.000	2000.000	33.000	0.400	0.010	0.017	24.340	35.060	0.075	1.610	0.100	0.050	0.001	0.110
3008.000	1800.000	148.000	0.070	0.009	0.016	25.180	35.250	0.710	1.690	0.040	0.040	0.001	0.080
5012.000	1700.000	32.000	0.070	0.009	0.016	25.180	35.250	0.710	1.690	0.040	0.040	0.001	0.080
3000.000	1750.000	838.000	0.130	0.009	0.018	24.270	34.140	0.730	1.630	0.090	0.020	0.001	0.040
6000.000	1600.000	140.000	0.110	0.009	0.019	24.240	34.280	0.690	1.640	0.090	0.020	0.001	0.004
4303.000	1700.000	471.000	0.110	0.008	0.017	24.190	34.180	0.800	1.640	0.080	0.030	0.001	0.040
2700.000	1742.000	424.000	0.080	0.006	0.019	23.210	34.330	0.840	1.650	0.020	0.010	0.001	0.020
2700.000	1742.000	424.000	0.080	0.006	0.109	23.210	34.330	0.840	1.650	0.020	0.010	0.001	0.020
6019.000	1700.000	50.000	0.160	0.010	0.018	25.350	34.830	1.000	1.770	0.080	0.050	0.001	0.040
2505.000	1900.000	246.000	0.180	0.010	0.017	24.770	35.320	0.990	1.760	0.080	0.050	0.001	0.040
3007.000	1800.000	1175.000	0.160	0.011	0.019	25.800	34.500	0.960	1.610	0.090	0.050	0.001	0.050
3998.000	1850.000	614.000	0.410	0.007	0.020	24.140	33.980	0.800	1.580	0.040	0.010	0.001	0.030
6120.000	1750.000	177.000	0.410	0.007	0.020	24.140	33.980	0.800	1.580	0.040	0.010	0.001	0.030
5003.000	1800.000	132.000	0.410	0.007	0.020	24.140	33.980	0.800	1.580	0.040	0.010	0.001	0.030
3560.000	1750.000	483.000	0.410	0.013	0.017	25.100	35.430	0.830	1.710	0.080	0.050	0.001	0.050
3516.000	1900.000	634.000	0.410	0.009	0.014	24.900	35.700	1.060	1.470	0.066	0.000	0.005	0.100
5013.000	1800.000	322.000	0.390	0.009	0.018	25.100	35.800	1.120	1.760	0.070	0.000	0.005	0.140
3015.000	1950.000	591.000	0.390	0.010	0.013	25.700	35.500	1.170	1.620	0.065	0.000	0.005	0.110
1550.000	1850.000	33.000	0.410	0.005	0.010	24.900	35.200	1.040	1.530	0.052	0.000	0.005	0.060
2994.000	1950.000	336.000	0.400	0.009	0.020	25.840	35.240	0.920	1.500	0.060	0.050	0.001	0.040
3002.000	1950.000	90.000	0.440	0.008	0.020	24.020	33.510	0.870	1.760	0.090	0.010	0.001	0.000
3007.000	1950.000	72.000	0.390	0.011	0.018	25.800	35.920	0.830	1.480	0.080	0.050	0.001	0.040
3015.000	1950.000	83.000	0.420	0.008	0.023	25.070	33.930	0.810	1.620	0.090	0.060	0.001	0.060
4502.000	1900.000	44.000	0.420	0.010	0.017	25.180	35.380	0.830	1.670	0.070	0.050	0.001	0.040
3512.000	1800.000	2436.000	0.460	0.013	0.020	24.380	35.130	0.790	0.850	0.090	0.050	0.001	0.060
5500.000	1850.000	294.000	0.450	0.012	0.018	24.790	34.570	0.830	0.840	0.018	0.060	0.001	0.090
4193.000	1800.000	1790.000	0.430	0.012	0.019	23.740	35.030	0.770	0.840	0.080	0.050	0.001	0.060
3015.000	1950.000	87.000	0.400	0.010	0.018	25.950	34.930	0.890	1.730	0.080	0.050	0.002	0.040
3007.000	1950.000	115.000	0.380	0.011	0.019	26.590	33.830	1.250	1.420	0.080	0.050	0.001	0.050
5972.000	1800.000	177.000	0.470	0.011	0.020	25.850	35.250	0.890	1.120	0.090	0.040	0.001	0.290
4565.000	1900.000	32.000	0.430	0.008	0.019	23.380	33.960	0.770	1.680	0.070	0.010	0.001	0.030
2813.000	1900.000	127.000	0.070	0.010	0.016	21.980	34.340	0.700	1.720	0.080	0.110	0.001	0.000
2819.000	1900.000	36.000	0.070	0.009	0.016	22.020	34.750	0.710	1.710	0.080	0.110	0.001	0.000
3569.000	1750.000	946.000	0.096	0.011	0.016	19.470	32.800	0.690	1.020	0.110	0.100	0.001	0.000
5981.000	1600.000	225.000	0.090	0.011	0.016	19.970	32.350	0.730	1.050	0.110	0.110	0.001	0.000
2984.000	1750.000	517.000	0.110	0.010	0.015	19.630	32.380	0.710	1.010	0.110	0.100	0.001	0.000
2005.000	1850.000	636.000	0.090	0.011	0.015	19.670	33.330	0.710	1.080	0.150	0.120	0.001	0.000
4034.000	1800.000	54.000	0.850	0.010	0.016	20.060	32.370	0.650	0.930	0.100	0.110	0.001	0.000
4500.000	1700.000	299.000	0.085	0.010	0.016	20.060	32.370	0.650	0.930	0.100	0.110	0.001	0.000
2240.000	1950.000	212.000	0.090	0.011	0.015	20.010	32.970	0.740	1.000	0.050	0.120	0.001	0.000
2005.000	2000.000	595.000	0.400	0.007	0.017	33.280	46.940	1.420	1.740	0.030	0.030	0.004	0.080
5995.000	1800.000	28.000	0.400	0.007	0.016	31.750	46.360	1.410	1.650	0.030	0.030	0.004	0.080

second.xls

PSI	DEGREE F	HOURS	C	S	P	Cr	Ni	Mn	Si	Cu	Mo	Pb	Co
3008.000	1800.000	148.000	0.070	0.009	0.016	25.180	35.250	0.710	1.690	0.040	0.040	0.001	0.080
5012.000	1700.000	32.000	0.070	0.009	0.016	25.180	35.250	0.710	1.690	0.040	0.040	0.001	0.080
3000.000	1750.000	838.000	0.130	0.009	0.018	24.270	34.140	0.730	1.630	0.090	0.020	0.001	0.040
6000.000	1600.000	140.000	0.110	0.009	0.019	24.240	34.280	0.690	1.640	0.090	0.020	0.001	0.004
4303.000	1700.000	471.000	0.110	0.008	0.017	24.190	34.180	0.800	1.640	0.080	0.030	0.001	0.040
2700.000	1742.000	424.000	0.080	0.006	0.019	23.210	34.330	0.840	1.650	0.020	0.010	0.001	0.020
6019.000	1700.000	50.000	0.160	0.010	0.018	25.350	34.830	1.000	1.770	0.080	0.050	0.001	0.040
2505.000	1900.000	246.000	0.180	0.010	0.017	24.770	35.320	0.990	1.760	0.080	0.050	0.001	0.040
3007.000	1800.000	1175.000	0.160	0.011	0.019	25.800	34.500	0.960	1.610	0.090	0.050	0.001	0.050
3998.000	1850.000	614.000	0.410	0.007	0.020	24.140	33.980	0.800	1.580	0.040	0.010	0.001	0.030
6120.000	1750.000	177.000	0.410	0.007	0.020	24.140	33.980	0.800	1.580	0.040	0.010	0.001	0.030
5003.000	1800.000	132.000	0.410	0.007	0.020	24.140	33.980	0.800	1.580	0.040	0.010	0.001	0.030
3560.000	1750.000	483.000	0.410	0.013	0.017	25.100	35.430	0.830	1.710	0.080	0.050	0.001	0.050
3516.000	1900.000	634.000	0.410	0.009	0.014	24.900	35.700	1.060	1.470	0.066	0.000	0.005	0.100
5013.000	1800.000	322.000	0.390	0.009	0.018	25.100	35.800	1.120	1.760	0.070	0.000	0.005	0.140
3015.000	1950.000	591.000	0.390	0.010	0.013	25.700	35.500	1.170	1.620	0.065	0.000	0.005	0.110
1550.000	1850.000	33.000	0.410	0.005	0.010	24.900	35.200	1.040	1.530	0.052	0.000	0.005	0.060
2994.000	1950.000	336.000	0.400	0.009	0.020	25.840	35.240	0.920	1.500	0.060	0.050	0.001	0.040
3002.000	1950.000	90.000	0.440	0.008	0.020	24.020	33.510	0.870	1.760	0.090	0.010	0.001	0.000
3007.000	1950.000	72.000	0.390	0.011	0.018	25.800	35.920	0.830	1.480	0.080	0.050	0.001	0.040
3015.000	1950.000	83.000	0.420	0.008	0.023	25.070	33.930	0.810	1.620	0.090	0.060	0.001	0.060
4502.000	1900.000	44.000	0.420	0.010	0.017	25.180	35.380	0.830	1.670	0.070	0.050	0.001	0.040
3512.000	1800.000	2436.000	0.460	0.013	0.020	24.380	35.130	0.790	0.850	0.090	0.050	0.001	0.060
5500.000	1850.000	294.000	0.450	0.012	0.018	24.790	34.570	0.830	0.840	0.018	0.060	0.001	0.090
4193.000	1800.000	1790.000	0.430	0.012	0.019	23.740	35.030	0.770	0.840	0.080	0.050	0.001	0.060
3015.000	1950.000	87.000	0.400	0.010	0.018	25.950	34.930	0.890	1.730	0.080	0.050	0.002	0.040
3007.000	1950.000	115.000	0.380	0.011	0.019	26.590	33.830	1.250	1.420	0.080	0.050	0.001	0.050
5972.000	1800.000	177.000	0.470	0.011	0.020	25.850	35.250	0.890	1.120	0.090	0.040	0.001	0.290
4565.000	1900.000	32.000	0.430	0.008	0.019	23.380	33.960	0.770	1.680	0.070	0.010	0.001	0.030
2813.000	1900.000	127.000	0.070	0.010	0.016	21.980	34.340	0.700	1.720	0.080	0.110	0.001	0.000
2819.000	1900.000	36.000	0.070	0.009	0.016	22.020	34.750	0.710	1.710	0.080	0.110	0.001	0.000
3569.000	1750.000	946.000	0.096	0.011	0.016	19.470	32.800	0.690	1.020	0.110	0.100	0.001	0.000
5981.000	1600.000	225.000	0.090	0.011	0.016	19.970	32.350	0.730	1.050	0.110	0.110	0.001	0.000
2984.000	1750.000	517.000	0.110	0.010	0.015	19.630	32.380	0.710	1.010	0.110	0.100	0.001	0.000
2005.000	1850.000	636.000	0.090	0.011	0.015	19.670	33.330	0.710	1.080	0.150	0.120	0.001	0.000
4500.000	1700.000	299.000	0.085	0.010	0.016	20.060	32.370	0.650	0.930	0.100	0.110	0.001	0.000
2240.000	1950.000	212.000	0.090	0.011	0.015	20.010	32.970	0.740	1.000	0.050	0.120	0.001	0.000
2005.000	2000.000	595.000	0.400	0.007	0.017	33.280	46.940	1.420	1.740	0.030	0.030	0.004	0.080
5995.000	1800.000	28.000	0.400	0.007	0.016	31.750	46.360	1.410	1.650	0.030	0.030	0.004	0.080
1600.000	1900.000	6331.000	0.370	0.009	0.018	34.340	45.420	1.040	1.300	0.020	0.020	0.004	0.080
1540.000	1900.000	10247.000	0.415	0.007	0.016	34.410	45.370	1.310	1.780	0.030	0.032	0.004	0.080
1796.000	2000.000	1297.000	0.424	0.008	0.016	32.650	44.610	1.370	1.710	0.040	0.032	0.004	0.080
3007.000	1900.000	474.000	0.402	0.008	0.018	33.770	45.530	1.330	1.610	0.030	0.034	0.005	0.080
1711.000	2075.000	140.000	0.420	0.005	0.016	35.280	45.170	1.510	1.810	0.040	0.026	0.004	0.090
1800.000	2000.000	434.000	0.440	0.007	0.018	32.820	43.920	1.380	1.910	0.030	0.030	0.005	0.090
3506.000	1850.000	183.000	0.433	0.007	0.016	32.370	45.090	1.340	1.710	0.040	0.032	0.004	0.090
1801.000	2000.000	534.000	0.400	0.007	0.016	32.080	45.570	1.270	1.710	0.040	0.030	0.004	0.080

task1.xls

Task1 results (3-criteria optimization)

predicted values

PSI	DEGREE F	HOURS	C	S	P	Cr	Ni	Mn	Si	Cu	Mo	Pb	Co
10026.000	1500.000	281.200	0.538	0.014	0.017	36.447	51.122	0.904	2.124	0.074	0.019	0.004	0.143
9904.000	1605.300	48.706	0.385	0.002	0.028	32.668	44.252	1.352	2.146	0.030	0.011	0.003	0.035
9784.200	1513.800	266.990	0.438	0.011	0.018	31.412	39.144	0.585	1.551	0.039	0.036	0.004	0.197
9673.300	1595.900	529.110	0.361	0.002	0.031	31.512	43.690	1.253	2.123	0.028	0.010	0.003	0.119
9652.700	1619.200	50.405	0.390	0.002	0.027	29.012	43.306	1.353	2.065	0.036	0.004	0.004	0.126
9572.200	1522.600	694.200	0.436	0.009	0.018	36.417	44.331	0.927	1.491	0.051	0.024	0.004	0.090
9507.400	1500.500	2206.500	0.206	0.001	0.031	33.271	34.496	0.673	1.246	0.028	0.031	0.005	0.112
9407.000	1589.200	1039.800	0.380	0.002	0.031	30.283	43.151	1.204	2.091	0.032	0.011	0.004	0.093
9324.200	1510.600	2336.700	0.266	0.005	0.028	30.759	36.054	0.811	1.246	0.034	0.019	0.005	0.085
9283.600	1639.800	47.878	0.424	0.001	0.025	33.941	42.592	1.513	2.107	0.031	0.011	0.003	0.068
9010.000	1527.000	2615.200	0.365	0.008	0.027	32.662	32.200	0.829	0.854	0.035	0.029	0.005	0.126
8948.300	1658.900	57.309	0.277	0.001	0.023	32.759	42.647	1.389	1.766	0.017	0.001	0.005	0.224
8873.700	1579.700	2056.200	0.377	0.002	0.030	30.446	43.111	1.192	2.097	0.029	0.009	0.004	0.095
8723.300	1659.000	597.530	0.391	0.002	0.027	27.386	41.571	1.228	1.961	0.038	0.002	0.005	0.162
8626.600	1547.200	2905.000	0.297	0.010	0.021	33.315	32.924	0.734	1.085	0.034	0.037	0.005	0.083
8448.100	1687.100	62.989	0.308	0.001	0.022	31.357	42.535	1.385	1.746	0.020	0.001	0.005	0.241
8269.500	1567.100	3210.100	0.382	0.006	0.023	28.820	32.699	0.738	1.161	0.047	0.021	0.005	0.117
8211.400	1588.800	1796.900	0.394	0.007	0.015	37.107	43.741	1.012	1.480	0.057	0.037	0.005	0.073
7852.200	1617.500	750.080	0.424	0.010	0.010	31.190	30.787	0.920	0.965	0.035	0.053	0.005	0.245
7839.100	1721.800	87.046	0.452	0.001	0.025	28.593	47.334	1.344	2.143	0.036	0.007	0.005	0.220
7773.600	1594.400	3772.500	0.504	0.012	0.031	37.092	22.335	0.669	0.605	0.061	0.002	0.005	0.113
7742.500	1612.300	2205.400	0.386	0.007	0.015	37.385	43.383	1.034	1.415	0.066	0.038	0.004	0.076
7679.000	1713.300	1046.900	0.408	0.002	0.027	26.755	41.150	1.278	1.902	0.041	0.000	0.005	0.172
7479.900	1742.000	78.522	0.454	0.001	0.025	27.513	47.439	1.418	2.148	0.033	0.006	0.004	0.220
7347.600	1616.200	4269.300	0.482	0.012	0.030	33.168	19.576	0.586	0.613	0.048	0.005	0.005	0.105
7095.000	1630.900	3458.700	0.444	0.014	0.022	32.770	39.724	1.120	0.528	0.017	0.056	0.005	0.163
7018.600	1748.200	1176.100	0.424	0.003	0.027	26.591	41.334	1.272	1.922	0.042	0.000	0.005	0.177
6951.800	1637.000	4506.900	0.479	0.013	0.029	32.796	19.442	0.607	0.615	0.044	0.002	0.005	0.093
6942.000	1658.700	2490.900	0.378	0.005	0.015	37.583	43.693	1.034	1.465	0.064	0.029	0.004	0.052
6928.500	1770.700	219.260	0.436	0.003	0.027	30.262	47.505	1.163	2.140	0.029	0.011	0.005	0.208
6701.300	1747.400	2307.700	0.425	0.003	0.027	26.577	41.088	1.247	1.892	0.041	0.001	0.005	0.177
6567.400	1790.900	228.650	0.433	0.001	0.029	30.775	48.076	1.116	2.146	0.032	0.006	0.005	0.215
6543.800	1658.900	4887.600	0.459	0.011	0.021	32.147	34.367	0.586	0.696	0.016	0.009	0.005	0.161
6216.900	1677.600	5398.100	0.469	0.012	0.026	37.684	30.185	0.730	0.605	0.037	0.007	0.004	0.093
6198.000	1805.100	622.650	0.463	0.002	0.026	29.804	47.702	1.142	2.145	0.028	0.011	0.005	0.203
5995.200	1774.400	3060.300	0.427	0.003	0.027	26.403	40.973	1.239	1.893	0.040	0.001	0.005	0.181
5904.400	1702.100	3822.500	0.379	0.007	0.015	37.687	43.153	1.026	1.405	0.064	0.036	0.004	0.073
5899.100	1829.000	204.060	0.455	0.002	0.028	31.724	48.259	1.159	2.149	0.029	0.012	0.005	0.206
5864.900	1695.500	5710.300	0.490	0.013	0.031	35.850	21.258	0.612	0.632	0.052	0.003	0.005	0.112
5692.400	1810.400	1953.000	0.457	0.002	0.028	27.300	46.506	1.130	2.127	0.031	0.009	0.005	0.207
5517.300	1714.300	6158.800	0.471	0.011	0.024	35.930	25.118	0.639	0.503	0.049	0.003	0.004	0.087
5448.200	1854.600	202.690	0.457	0.002	0.028	32.227	49.754	1.139	2.145	0.028	0.011	0.005	0.203
5081.600	1743.300	4583.200	0.367	0.007	0.017	36.489	42.305	0.941	1.375	0.052	0.029	0.005	0.080
5031.900	1741.100	6677.800	0.477	0.013	0.025	37.771	30.270	0.739	0.554	0.041	0.010	0.004	0.092
4990.400	1880.800	177.490	0.461	0.003	0.028	33.048	48.865	1.150	2.147	0.029	0.012	0.005	0.204

task2-6.xls

Task2 results (T>=1600)

predicted values

PSI	DEGREE F	HOURS	C	S	P	Cr	Ni	Mn	Si	Cu	Mo	Pb	Co
9965.300	1602.100	46.514	0.250	0.007	0.026	35.354	51.371	1.663	2.149	0.036	0.007	0.003	0.070
9637.800	1612.800	244.490	0.400	0.002	0.029	27.692	41.347	1.285	2.141	0.035	0.005	0.004	0.114
9340.700	1611.000	736.510	0.417	0.002	0.030	31.102	47.896	1.212	1.990	0.035	0.004	0.004	0.095
9078.300	1613.300	1216.600	0.406	0.003	0.029	29.749	43.656	1.195	2.083	0.034	0.005	0.003	0.145
8642.000	1610.200	1836.600	0.358	0.002	0.029	30.188	44.275	1.165	2.001	0.034	0.005	0.003	0.119
8212.700	1616.700	2433.400	0.383	0.003	0.029	30.050	43.051	1.099	2.150	0.034	0.006	0.003	0.132
7818.800	1625.800	2862.900	0.373	0.003	0.030	28.648	42.234	1.179	2.068	0.035	0.005	0.004	0.109
7647.300	1600.000	3969.200	0.476	0.012	0.030	32.423	21.258	0.585	0.645	0.050	0.005	0.005	0.100
6766.700	1647.300	4882.100	0.475	0.013	0.029	35.390	23.643	0.728	0.668	0.045	0.004	0.004	0.094
6427.400	1665.500	5239.100	0.479	0.013	0.028	35.184	24.357	0.714	0.625	0.044	0.004	0.004	0.096
5694.100	1704.900	5996.100	0.485	0.014	0.028	34.882	23.848	0.707	0.563	0.045	0.004	0.004	0.104
5264.900	1727.900	6437.600	0.484	0.014	0.027	35.093	24.183	0.702	0.579	0.044	0.005	0.004	0.107
4716.200	1757.600	7043.100	0.480	0.014	0.026	36.863	26.335	0.763	0.574	0.041	0.004	0.004	0.106
4230.900	1783.600	7526.900	0.493	0.014	0.026	35.402	25.756	0.698	0.531	0.042	0.005	0.004	0.118
3571.600	1818.700	8122.100	0.485	0.014	0.024	35.675	27.140	0.690	0.533	0.042	0.005	0.004	0.116
3075.100	1845.700	8702.500	0.487	0.013	0.021	37.782	29.576	0.682	0.479	0.038	0.007	0.004	0.123
2733.500	1864.700	9205.500	0.494	0.014	0.022	36.612	30.010	0.686	0.470	0.037	0.007	0.004	0.127
2279.200	1889.900	9824.400	0.497	0.014	0.019	37.886	34.216	0.685	0.426	0.034	0.009	0.004	0.130
2068.100	1902.200	10244.000	0.508	0.014	0.019	37.279	35.911	0.696	0.512	0.039	0.010	0.004	0.136
1706.100	1923.500	10946.000	0.519	0.013	0.015	39.290	41.969	0.691	0.188	0.020	0.013	0.004	0.120

Task3 results (T>=1800)

predicted values

PSI	DEGREE F	HOURS	C	S	P	Cr	Ni	Mn	Si	Cu	Mo	Pb	Co
6425.400	1800.000	191.530	0.473	0.002	0.026	31.058	48.328	1.106	2.149	0.027	0.010	0.005	0.220
6261.900	1801.400	623.750	0.466	0.002	0.027	29.218	47.718	1.127	2.150	0.028	0.011	0.005	0.210
5956.800	1814.300	862.010	0.466	0.002	0.026	29.591	47.668	1.143	2.144	0.029	0.010	0.005	0.204
5949.700	1800.300	1675.100	0.455	0.002	0.028	27.377	46.291	1.140	2.135	0.030	0.009	0.005	0.208
5669.800	1801.000	2577.800	0.437	0.002	0.026	27.009	41.617	1.153	1.920	0.044	0.001	0.005	0.182
5405.900	1807.500	3107.300	0.435	0.003	0.026	27.038	41.715	1.138	1.919	0.045	0.001	0.005	0.180
5115.100	1809.000	4013.900	0.426	0.003	0.027	25.993	40.845	1.224	1.881	0.041	0.000	0.005	0.174
4762.700	1821.700	4434.500	0.425	0.003	0.027	25.728	40.685	1.227	1.891	0.042	0.000	0.005	0.172
4366.100	1837.000	4860.200	0.425	0.003	0.027	25.716	40.801	1.220	1.890	0.041	0.000	0.005	0.172
4015.000	1849.500	5228.400	0.422	0.003	0.028	25.223	40.455	1.239	1.880	0.041	0.000	0.005	0.171
3937.300	1800.000	7931.200	0.468	0.014	0.024	36.992	23.732	0.678	0.622	0.039	0.013	0.004	0.139
3735.000	1810.800	8101.800	0.467	0.014	0.024	37.436	24.445	0.693	0.562	0.039	0.011	0.004	0.142
3422.000	1828.000	8561.900	0.451	0.014	0.024	38.955	24.452	0.644	0.660	0.042	0.015	0.005	0.138
3086.900	1845.800	8807.500	0.480	0.014	0.024	37.627	27.069	0.670	0.513	0.034	0.010	0.004	0.152
2818.900	1860.300	9134.700	0.477	0.014	0.023	37.499	25.902	0.692	0.552	0.043	0.015	0.004	0.141
2617.900	1872.400	9618.800	0.483	0.014	0.023	38.635	29.616	0.749	0.453	0.032	0.012	0.004	0.128
2356.200	1886.400	9905.300	0.484	0.014	0.022	38.841	29.712	0.680	0.450	0.035	0.013	0.004	0.133
2064.100	1902.800	10323.000	0.492	0.014	0.020	38.913	30.629	0.680	0.461	0.031	0.011	0.004	0.127
1847.800	1915.100	10693.000	0.508	0.014	0.018	38.920	35.082	0.672	0.304	0.024	0.010	0.004	0.125
1721.100	1923.100	10941.000	0.526	0.013	0.016	39.529	43.995	0.676	0.219	0.021	0.012	0.004	0.111

derivatives.xls

examples of the derivatives evaluation

	PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W	Ti
point	2930.400	2000.000	789.100	0.469	34.020	43.830	1.457	0.151	0.000	1.293	0.019	0.002
d(PSI)/dx				-1072.000	6.188	-24.940	-987.700	10.910	-304.200	317.900	-157.200	31830.000
d(temp)/dx				78.260	-0.016	2.795	66.030	-10.980	-38.010	-25.170	19.880	-3529.000
d(HOURS)/dx)				-484.100	3.040	-39.540	-954.400	-7.244	459.400	-36.990	-49.550	54850.000
point	2765.500	2000.400	1575.800	0.485	32.010	38.160	1.311	0.131	0.001	0.865	0.236	0.002
d(PSI)/dx				-695.800	0.199	-14.190	-349.500	96.330	46.940	306.900	-226.100	18770.000
d(temp)/dx				56.660	-0.310	2.811	97.040	-3.788	-8.015	-20.110	26.840	-3150.000
d(HOURS)/dx)				-274.100	20.940	-92.200	-3993.000	-305.100	-45.180	-308.200	3.188	91230.000
point	1913.700	2000.000	3190.500	0.475	35.450	48.050	0.985	2.137	0.013	0.612	0.461	0.017
d(PSI)/dx				-2997.000	65.510	16.670	1368.000	107.700	-1144.000	-823.200	95.550	8023.000
d(temp)/dx				-170.500	11.820	1.585	109.900	1.660	271.600	-114.300	-52.180	-260.300
d(HOURS)/dx)				22780.000	-893.400	-164.700	-11350.000	-508.100	-12890.000	8524.000	2208.000	-34190.000
point	2445.600	2050.000	156.900	0.216	39.280	44.170	1.468	1.651	0.128	1.125	0.085	0.070
d(PSI)/dx				2630.000	-7.484	-6.102	-584.400	669.700	-1590.000	153.000	1248.000	-3509.000
d(temp)/dx				-218.700	1.626	0.685	69.730	-56.320	144.000	-39.250	-91.230	297.600
d(HOURS)/dx)				482.300	-11.000	-6.092	-579.700	120.400	-487.200	559.300	-22.270	284.400
point	2296.100	2050.300	495.200	0.208	39.360	43.960	1.398	1.877	0.129	1.191	0.065	0.072
d(PSI)/dx				1900.000	-10.130	-2.719	-340.800	499.300	-1192.000	52.970	977.400	-2581.000
d(temp)/dx				-222.600	3.349	1.042	113.300	-58.660	171.800	-91.380	-72.940	217.200
d(HOURS)/dx)				2227.000	-39.400	-28.630	-2816.000	568.600	-2230.000	2616.000	-98.480	3323.000
point	2131.800	2050.500	883.900	0.259	39.530	45.820	1.341	1.339	0.127	1.182	0.107	0.086
d(PSI)/dx				1106.000	-7.663	-2.077	-284.500	266.600	-812.500	37.930	637.300	-2561.000
d(temp)/dx				-134.600	3.084	1.588	279.000	-11.400	465.600	-148.500	-44.540	-52.820
d(HOURS)/dx)				1799.000	-71.480	-51.120	-7884.000	-83.900	-10410.000	4921.000	-46.350	8276.000
point	1923.900	2050.000	1155.000	0.266	39.570	47.870	1.365	1.062	0.127	1.093	0.068	0.085
d(PSI)/dx				439.900	0.655	-2.716	-197.100	87.950	-422.800	85.760	141.200	-1807.000
d(temp)/dx				111.400	3.287	2.590	725.000	128.600	1393.000	-246.500	-7.686	-410.800
d(HOURS)/dx)				-3540.000	-88.610	-64.530	-18350.000	-3437.000	-34030.000	6333.000	-32.070	13280.000

distan.xls

PSI	DEGREE F	HOURS	C	S	P	Cr	Ni	Mn	Si	Cu	Mo	Pb	Co
10023.000	1600.000	23.000	0.120	0.008	0.019	33.930	44.590	0.910	1.450	0.040	0.020	0.004	0.240
6030.000	1800.000	13.000	0.120	0.008	0.019	33.930	44.590	0.910	1.450	0.040	0.020	0.004	0.240
1275.000	1950.000	12176.000	0.390	0.009	0.018	34.790	44.680	1.020	1.310	0.020	0.020	0.004	0.080
9516.000	1500.000	2200.000	0.380	0.008	0.019	34.760	44.700	1.030	1.340	0.020	0.020	0.004	0.080
3512.000	1800.000	2436.000	0.460	0.013	0.020	24.380	35.130	0.790	0.850	0.090	0.050	0.001	0.060
5521.000	1850.000	106.000	0.460	0.011	0.019	24.360	35.100	0.830	0.840	0.090	0.050	0.001	0.060
9516.000	1500.000	2200.000	0.380	0.008	0.019	34.760	44.700	1.030	1.340	0.020	0.020	0.004	0.080
5303.000	1700.000	1536.000	0.390	0.009	0.018	34.740	44.600	1.020	1.340	0.020	0.020	0.004	0.080
2500.000	2050.000	18.000	0.390	0.009	0.018	34.680	45.810	1.080	1.330	0.020	0.020	0.004	0.080
3007.000	1800.000	10646.000	0.380	0.009	0.018	34.660	45.710	1.130	1.330	0.020	0.020	0.004	0.080

Appendix 2

v9-task1-3criteria.xls

Task1 results (9 variables, 3-criteria optimization)

predicted values

PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W	Ti
8274.310	1703.650	663.147	0.600	17.561	35.000	2.000	2.000	0.025	0.947	0.328	0.053
8129.430	1710.150	630.976	0.600	17.501	34.991	2.000	1.965	0.000	0.847	0.412	0.066
7931.390	1709.050	764.192	0.473	17.501	34.995	1.974	1.740	0.000	0.077	0.026	0.008
7810.760	1723.040	606.118	0.489	17.586	34.987	1.994	1.990	0.002	0.565	0.359	0.056
7647.530	1714.990	814.611	0.382	21.811	34.009	1.996	0.899	0.164	0.081	0.159	0.042
7506.380	1736.980	557.099	0.490	17.581	34.986	1.990	1.961	0.001	0.429	0.331	0.052
7255.740	1717.120	984.422	0.115	18.890	35.000	1.879	1.987	0.036	0.003	0.094	0.009
7236.600	1750.220	492.057	0.507	17.608	34.989	1.994	1.994	0.001	0.621	0.415	0.062
7028.240	1720.810	1045.850	0.096	19.077	35.000	1.857	1.984	0.039	0.002	0.051	0.009
6920.060	1765.040	437.159	0.492	17.521	35.000	2.000	1.993	0.003	0.490	0.403	0.057
6894.960	1756.870	842.302	0.459	28.418	34.855	2.000	0.505	0.044	0.797	0.236	0.106
6578.800	1780.680	379.374	0.482	17.579	34.987	1.993	1.973	0.000	0.560	0.378	0.067
6550.480	1732.950	1103.230	0.107	29.988	34.876	1.997	0.099	0.019	0.335	0.144	0.002
6339.560	1764.400	1306.050	0.110	29.423	34.907	1.566	0.414	0.014	1.750	0.047	0.103
6246.240	1796.270	319.820	0.479	17.588	34.986	1.993	1.982	0.001	0.481	0.347	0.068
6101.700	1800.080	1002.590	0.467	28.388	34.846	1.999	0.487	0.040	0.838	0.233	0.108
6095.890	1682.900	3301.220	0.591	29.737	34.873	1.061	0.629	0.012	2.977	0.149	0.051
6067.340	1774.510	1559.290	0.112	29.440	34.912	1.569	0.416	0.014	1.754	0.046	0.111
5973.000	1689.870	3490.630	0.593	29.729	34.860	1.068	0.625	0.010	2.959	0.152	0.066
5928.580	1811.050	597.233	0.432	27.984	34.814	2.000	0.473	0.039	0.660	0.190	0.115
5877.140	1703.270	3039.180	0.591	29.757	34.880	1.088	0.637	0.013	2.973	0.150	0.035
5761.330	1785.590	1865.250	0.113	29.424	34.939	1.581	0.411	0.013	1.789	0.041	0.115
5747.020	1700.000	3562.820	0.565	29.797	34.418	0.911	0.970	0.015	2.654	0.117	0.072
5736.820	1820.250	222.693	0.481	17.589	34.984	1.994	1.989	0.000	0.484	0.429	0.064
5693.350	1719.870	2876.750	0.592	29.759	34.881	1.083	0.633	0.013	2.971	0.150	0.029
5546.560	1717.740	3705.100	0.591	29.756	34.866	1.103	0.510	0.011	2.868	0.155	0.074
5504.470	1737.510	2706.010	0.592	29.757	34.883	1.084	0.633	0.014	2.969	0.151	0.025
5486.630	1795.400	2137.350	0.116	29.474	34.926	1.587	0.416	0.014	1.764	0.048	0.116
5475.820	1836.500	528.504	0.432	27.789	34.818	2.000	0.401	0.037	0.652	0.177	0.118
5388.640	1808.900	1257.440	0.097	29.219	34.838	1.681	0.395	0.009	1.550	0.005	0.066
5211.910	1765.240	2516.080	0.592	29.724	34.871	1.127	0.637	0.014	2.893	0.158	0.022
5210.020	1734.900	3903.080	0.568	29.817	34.541	1.031	0.902	0.016	2.453	0.136	0.076
5102.560	1850.110	109.813	0.322	29.948	35.000	1.991	0.224	0.002	0.402	0.160	0.114
5033.020	1751.660	3505.250	0.498	29.794	34.265	0.875	1.134	0.020	2.218	0.103	0.071
5028.200	1812.180	2607.820	0.117	29.459	34.956	1.604	0.414	0.014	1.835	0.044	0.126
4977.350	1744.590	3962.320	0.565	29.759	34.498	0.931	0.932	0.017	2.534	0.113	0.093
4913.550	1874.080	677.530	0.432	27.765	34.807	2.000	0.436	0.037	0.689	0.176	0.117
4789.680	1875.170	193.954	0.322	29.912	34.967	1.983	0.238	0.002	0.491	0.142	0.096
4768.270	1786.700	3308.170	0.588	29.715	34.823	1.323	0.346	0.016	2.650	0.172	0.054
4737.330	1875.650	1271.080	0.465	28.352	34.856	2.000	0.515	0.040	0.854	0.225	0.111
4673.030	1761.790	4092.990	0.546	29.777	34.352	0.920	1.054	0.018	2.344	0.111	0.095
4656.170	1838.600	1821.900	0.104	29.155	34.867	1.695	0.395	0.009	1.566	0.015	0.070
4565.810	1829.350	3059.410	0.118	29.368	34.961	1.638	0.410	0.013	1.791	0.038	0.124
4474.440	1796.310	3955.930	0.588	29.741	34.829	1.295	0.400	0.014	2.596	0.176	0.076
4356.820	1906.820	149.790	0.325	30.000	34.981	1.979	0.243	0.002	0.400	0.106	0.099

v9-task2-6.xls

9 variables, 2 criteria

Task2 results (T>=1700)

predicted values

PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W	Ti
8275.420	1703.680	662.202	0.600	17.501	34.997	2.000	2.000	0.027	0.891	0.338	0.050
8023.120	1706.750	745.831	0.296	17.500	35.000	2.000	2.000	0.034	0.103	0.202	0.000
7697.490	1711.600	838.384	0.309	19.036	34.969	1.886	1.964	0.032	0.355	0.181	0.000
7129.080	1720.120	1002.590	0.263	20.558	34.956	1.788	1.911	0.031	0.391	0.138	0.008
6797.450	1725.080	1099.440	0.172	20.253	34.929	1.771	1.842	0.035	0.142	0.111	0.000
6412.000	1762.290	1217.630	0.108	29.434	34.919	1.558	0.417	0.014	1.764	0.045	0.110
6121.770	1772.620	1511.750	0.109	29.435	34.928	1.578	0.400	0.014	1.762	0.042	0.111
5913.620	1779.810	1713.890	0.115	29.443	34.925	1.566	0.404	0.014	1.756	0.043	0.111
5913.110	1700.010	3067.320	0.590	29.757	34.882	1.082	0.634	0.013	2.976	0.149	0.036
5850.120	1700.500	3307.400	0.588	29.811	34.632	1.063	0.678	0.014	2.823	0.139	0.048
5635.270	1712.710	3644.060	0.589	29.800	34.611	1.118	0.674	0.015	2.769	0.157	0.066
5307.990	1731.610	3803.440	0.527	29.830	34.470	1.088	1.000	0.016	2.314	0.131	0.059
5035.530	1748.000	3956.990	0.524	29.829	34.471	1.096	0.974	0.016	2.228	0.129	0.066
4474.810	1778.190	4223.300	0.488	29.802	34.473	1.068	1.039	0.018	2.042	0.106	0.079
4013.080	1795.190	4288.180	0.536	29.761	34.240	0.814	1.120	0.019	2.240	0.085	0.112
3575.970	1818.270	4417.390	0.555	29.735	34.237	0.773	1.119	0.020	2.347	0.079	0.130
3184.930	1842.420	4555.500	0.538	29.742	34.237	0.828	1.130	0.020	2.137	0.079	0.136
2792.840	1858.490	4665.120	0.562	29.657	34.232	0.684	1.124	0.021	2.379	0.075	0.162
2481.880	1873.330	4765.630	0.571	29.650	34.206	0.620	1.119	0.022	2.361	0.059	0.181
2131.870	1885.280	4884.960	0.576	29.639	34.150	0.380	1.080	0.024	2.454	0.031	0.205

Task3 results (T>=1800)

predicted values

PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W	Ti
6141.080	1800.010	901.859	0.460	28.381	34.842	2.000	0.491	0.041	0.794	0.223	0.108
6041.130	1800.310	1127.780	0.477	28.315	34.837	1.998	0.490	0.037	0.880	0.243	0.110
5796.800	1813.340	1188.730	0.478	28.287	34.838	2.000	0.473	0.038	0.878	0.239	0.110
5506.780	1827.620	1309.470	0.482	28.286	34.837	1.998	0.488	0.037	0.892	0.239	0.110
5505.600	1800.000	1631.640	0.097	29.213	34.839	1.688	0.393	0.010	1.555	0.006	0.077
5409.520	1800.010	2075.810	0.101	29.219	34.907	1.671	0.397	0.014	1.721	0.020	0.094
5324.280	1801.690	2279.310	0.110	29.263	34.861	1.635	0.401	0.012	1.761	0.024	0.105
5107.830	1808.360	2520.120	0.123	29.601	34.999	1.568	0.399	0.023	2.055	0.052	0.114
4867.160	1816.810	2761.960	0.127	29.574	34.994	1.568	0.404	0.023	2.055	0.055	0.114
4559.610	1827.700	3090.900	0.132	29.657	35.000	1.558	0.404	0.026	2.143	0.062	0.124
4249.600	1838.450	3431.950	0.139	29.706	35.000	1.547	0.407	0.029	2.244	0.071	0.131
4249.580	1800.000	4071.930	0.529	29.891	34.183	1.132	1.203	0.021	2.197	0.087	0.089
4019.050	1800.000	4302.840	0.541	29.757	34.246	0.922	1.165	0.020	2.193	0.098	0.109
3776.290	1810.390	4372.190	0.539	29.727	34.252	0.852	1.165	0.020	2.230	0.102	0.119
3472.350	1823.500	4456.070	0.548	29.692	34.265	0.759	1.150	0.020	2.282	0.100	0.131
3005.130	1844.610	4591.870	0.563	29.645	34.270	0.634	1.107	0.020	2.344	0.075	0.150
2730.370	1857.570	4682.780	0.562	29.604	34.271	0.573	1.108	0.020	2.362	0.086	0.161
2525.750	1866.260	4741.220	0.568	29.560	34.232	0.473	1.117	0.022	2.467	0.059	0.174
2313.750	1876.830	4828.410	0.572	29.578	34.187	0.453	1.088	0.023	2.457	0.051	0.188
2138.880	1885.150	4881.980	0.579	29.609	34.166	0.389	1.085	0.023	2.459	0.037	0.206

v8-task1-3criteria.xls

Task1 results (8 variables, 3-criteria optimization)

predicted values

PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W
8248.570	1704.120	668.905	0.600	29.929	34.267	2.000	2.000	0.130	1.006	0.428
8144.770	1708.140	648.721	0.596	29.871	34.680	1.983	2.000	0.127	0.768	0.646
7923.950	1719.370	660.519	0.596	29.960	33.687	1.997	1.965	0.125	0.510	0.206
7822.790	1711.580	766.137	0.527	28.607	34.239	1.828	1.872	0.147	0.617	0.387
7710.620	1730.670	638.267	0.598	29.961	33.662	1.997	1.955	0.126	0.516	0.198
7635.370	1715.210	814.950	0.412	29.913	34.902	2.000	0.704	0.071	0.553	0.230
7524.770	1740.580	618.000	0.597	29.960	33.560	1.998	1.946	0.125	0.518	0.191
7424.140	1717.180	896.306	0.163	29.962	34.999	1.992	1.269	0.128	0.261	0.197
7306.380	1752.220	594.266	0.597	29.958	33.579	1.997	1.946	0.126	0.516	0.186
7203.630	1721.320	943.310	0.218	30.000	35.000	1.922	1.159	0.141	0.223	0.204
7066.010	1765.250	565.428	0.598	29.940	33.594	2.000	1.954	0.126	0.516	0.182
6860.370	1747.030	604.542	0.095	26.231	33.564	1.913	1.491	0.116	0.157	0.747
6785.340	1742.660	869.508	0.529	29.661	34.801	1.915	0.298	0.000	0.058	0.017
6777.630	1726.720	1050.210	0.022	26.251	33.147	1.797	1.823	0.139	0.037	0.367
6776.510	1780.610	534.999	0.597	29.962	33.595	1.997	1.951	0.126	0.516	0.178
6531.730	1793.850	503.541	0.597	29.933	33.567	1.999	1.967	0.124	0.514	0.174
6414.120	1736.630	1105.390	0.151	27.524	33.814	1.763	1.029	0.179	0.001	0.235
6334.730	1804.320	485.062	0.597	29.959	33.615	1.997	1.951	0.126	0.515	0.172
6168.210	1741.250	1180.100	0.116	29.744	33.936	1.851	0.361	0.071	0.126	0.137
6066.700	1818.460	455.538	0.596	29.972	33.581	1.997	1.960	0.125	0.528	0.172
6017.910	1759.060	939.977	0.340	24.097	34.091	1.469	0.974	0.198	0.000	0.389
5870.780	1830.610	416.898	0.595	29.948	33.416	1.998	1.926	0.124	0.381	0.130
5832.970	1746.530	1283.430	0.034	29.620	33.195	1.861	0.069	0.022	0.077	0.070
5807.550	1802.390	609.827	0.301	29.690	34.441	1.991	0.844	0.173	0.228	0.136
5633.480	1772.370	1054.550	0.123	29.826	32.783	1.878	0.038	0.111	0.125	0.102
5617.510	1750.950	1329.860	0.001	29.725	33.125	1.812	0.021	0.002	0.067	0.044
5605.550	1843.270	405.104	0.598	29.964	33.601	1.998	1.949	0.126	0.526	0.166
5299.080	1812.460	827.645	0.560	28.779	34.902	1.440	1.421	0.015	0.223	0.017
5274.540	1863.110	346.450	0.596	29.947	33.524	1.996	1.926	0.125	0.388	0.125
5248.610	1760.990	1291.260	0.000	29.724	33.086	1.680	0.001	0.001	0.014	0.014
5026.930	1766.190	1237.520	0.000	29.805	33.044	1.656	0.014	0.007	0.025	0.019
5021.020	1876.880	313.182	0.596	29.955	33.409	1.996	1.935	0.124	0.384	0.121
5011.280	1843.960	474.805	0.309	29.605	34.467	1.983	0.858	0.172	0.240	0.126
4898.060	1843.260	799.489	0.567	28.636	34.904	1.438	1.436	0.015	0.275	0.015
4803.490	1773.080	1176.640	0.003	29.850	33.002	1.648	0.002	0.012	0.001	0.005
4796.310	1884.170	175.736	0.523	29.065	34.899	1.697	1.494	0.000	0.205	0.016
4688.130	1806.950	1246.470	0.588	27.301	26.373	0.001	0.234	0.043	2.005	0.295
4566.720	1871.860	743.104	0.569	28.962	34.911	1.414	1.506	0.017	0.273	0.014
4510.460	1905.150	256.458	0.578	29.825	33.558	1.967	1.778	0.110	0.298	0.082
4485.580	1806.270	1448.400	0.597	27.367	25.000	0.005	0.200	0.046	2.322	0.261
4442.960	1833.930	1624.430	0.573	29.717	34.985	1.119	1.358	0.000	1.654	0.000
4408.660	1831.300	1847.040	0.568	29.786	34.985	1.141	1.357	0.001	1.641	0.001
4307.460	1881.030	349.177	0.391	28.979	34.783	1.932	0.878	0.187	0.308	0.140
4279.590	1914.780	80.580	0.599	29.431	33.770	1.818	1.773	0.002	0.224	0.001
4110.920	1844.570	2114.010	0.576	29.599	34.985	1.171	1.357	0.000	1.606	0.000

v8-task2-6.xls

8 variables, 2 criteria

Task2 results (T>=1700)

predicted values

PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W
8248.750	1704.130	668.672	0.600	29.884	34.281	2.000	2.000	0.129	1.018	0.428
8000.820	1708.470	725.090	0.413	29.085	34.573	2.000	1.498	0.172	0.710	0.379
7734.930	1712.260	801.385	0.337	28.767	34.538	1.917	1.653	0.164	0.569	0.343
7310.130	1717.640	931.917	0.198	27.649	34.484	1.825	1.962	0.159	0.370	0.327
6736.920	1725.750	1097.380	0.095	27.222	34.191	1.744	1.934	0.134	0.204	0.296
6312.590	1733.060	1202.470	0.050	27.075	33.948	1.689	1.762	0.123	0.044	0.258
5796.400	1745.440	1269.060	0.014	26.499	33.761	1.588	1.341	0.095	0.052	0.253
5503.170	1753.510	1345.360	0.000	29.176	33.201	1.753	0.001	0.000	0.076	0.045
4961.220	1792.520	1662.750	0.580	30.000	34.985	1.038	1.355	0.000	2.455	0.001
4744.980	1808.150	1795.980	0.578	29.983	34.985	1.121	1.355	0.000	1.867	0.000
4530.120	1821.410	1987.860	0.579	29.966	34.985	1.144	1.356	0.000	1.638	0.000
4227.930	1834.170	2271.190	0.582	29.865	34.985	1.171	1.356	0.000	1.621	0.000
3991.870	1845.820	2505.260	0.585	29.809	34.985	1.190	1.357	0.000	1.537	0.000
3788.570	1855.190	2647.330	0.585	29.749	34.985	1.207	1.357	0.000	1.523	0.000
3578.670	1864.560	2874.690	0.595	29.618	34.985	1.223	1.359	0.000	1.510	0.000
3334.390	1876.230	3168.740	0.598	29.606	34.985	1.246	1.360	0.000	1.410	0.000
3172.780	1883.770	3343.890	0.600	29.603	34.985	1.264	1.361	0.001	1.355	0.000
2981.340	1893.640	3649.820	0.600	29.762	34.985	1.284	1.362	0.001	1.191	0.000
2910.290	1897.950	3826.280	0.600	29.982	34.986	1.289	1.364	0.001	1.076	0.000
2739.240	1909.360	3901.340	0.600	30.000	34.986	1.312	1.364	0.001	0.967	0.000

Task3 results (T>=1800)

predicted values

PSI	DEGREE F	HOURS	C	Cr	Ni	Mn	Si	Mo	Cb	W
6418.850	1800.010	493.920	0.599	29.963	33.623	2.000	1.939	0.125	0.514	0.172
6225.470	1800.090	572.903	0.592	29.989	33.767	1.871	1.878	0.124	0.572	0.179
5875.360	1800.090	606.422	0.311	29.701	34.474	1.997	0.862	0.175	0.242	0.140
5671.190	1800.040	718.373	0.548	29.207	34.915	1.533	1.467	0.019	0.089	0.009
5451.030	1800.200	826.364	0.550	29.195	34.917	1.486	1.471	0.020	0.002	0.009
5140.440	1804.740	828.854	0.587	27.375	26.602	0.000	0.161	0.047	2.014	0.302
4939.320	1805.790	1014.230	0.587	27.376	26.569	0.003	0.197	0.045	2.002	0.301
4939.300	1800.010	1631.260	0.589	30.000	34.985	1.091	1.360	0.000	1.907	0.000
4853.750	1802.230	1778.200	0.588	30.000	34.985	1.113	1.360	0.000	1.878	0.000
4585.920	1815.270	2069.250	0.587	30.000	34.985	1.145	1.360	0.000	1.701	0.000
4407.900	1825.140	2318.330	0.598	29.999	34.985	1.160	1.356	0.000	1.555	0.000
4213.520	1832.240	2572.510	0.600	30.000	34.985	1.178	1.356	0.000	1.547	0.000
4022.590	1840.150	2753.700	0.600	30.000	34.985	1.193	1.356	0.000	1.544	0.000
3774.860	1851.520	2955.990	0.600	29.999	34.985	1.213	1.355	0.000	1.517	0.000
3609.410	1859.770	3108.980	0.600	29.996	34.985	1.226	1.354	0.000	1.463	0.000
3427.430	1868.780	3288.330	0.600	29.996	34.985	1.242	1.356	0.000	1.397	0.000
3258.610	1877.950	3506.670	0.600	29.996	34.985	1.257	1.358	0.000	1.278	0.000
3130.070	1885.290	3656.060	0.600	29.994	34.985	1.268	1.359	0.000	1.184	0.000
2907.130	1898.370	3849.500	0.600	29.997	34.984	1.291	1.365	0.000	1.048	0.000
2750.950	1908.730	3896.630	0.600	29.997	34.984	1.312	1.364	0.000	0.964	0.000